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NUCLEAR ENERGY AGENCY
COMMITTEE ON THE SAFETY OF NUCLEAR INSTALLATIONS

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Working Group on the Analysis and Management of Accidents

(TECHNICAL NOTE)

ASSESSMENT OF CFD CODES FOR NUCLEAR REACTOR SAFETY PROBLEMS

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COMMITTEE ON THE SAFETY OF NUCLEAR INSTALLATIONS

WORKING GROUP ON THE ANALYSIS AND MANAGEMENT OF ACCIDENTS

The Working Group on the Analysis and Management of Accidents (GAMA) is mainly composed of technical specialists in the areas of thermal-hydraulics of the reactor coolant system and related safety and auxiliary systems, in-vessel behaviour of degraded cores and in-vessel protection, containment behaviour and containment protection, and fission product release, transport, deposition and retention. Its general functions include the exchange of information on national and international activities in these areas, the exchange of detailed technical information, and the discussion of progress achieved in respect of specific technical issues. Severe accident management is one of the important tasks of the group.

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EXECUTIVE SUMMARY

Background

This activity was undertaken in response to an initiative taken at the “Exploratory Meeting of Experts to Define an Action Plan on the Application of Computational Fluid Dynamics (CFD) Codes to Nuclear Reactor Safety Problems”, held at Aix-en-Provence, France, 15-16 May, 2002, and summarised in document NEA/SEN/SIN/AMA(2002)15. At this meeting, there was a consensus among the delegates to (1) provide a set of guidelines for the application of CFD to Nuclear Reactor Safety (NRS) problems; (2) to evaluate the existing CFD assessment basis and identify gaps that need to be filled in order to adequately validate CFD codes for application to NRS problems; and (3) to summarise the extensions needed to CFD codes for application to two-phase NRS problems. Three Writing Groups were formed in response to these initiatives; the present summary document focuses on the second of these.

Objectives

The group (WG2) set itself the following objectives:

- to review critically those NRS problems where the use of CFD is needed for the analysis, or where its use is expected to result in major benefits;
- to review critically the existing assessment basis for CFD application to NRS issues;
- to identify the gaps in the technology base, and the need for further development effort; and
- to propose a methodology for establishing assessment matrices relevant to NRS needs.

Procedure

Meetings were held on four occasions during the period March 2003 to June 2004. During the first of these meetings, the principal subject headings were identified, broadly following the objectives listed above. Tasks were assigned to each group member to supply expert information in specific subject areas, and deadlines for submission of material set. As a result, an action list containing 86 items was drawn up. From information supplied as a result of these actions, a first draft of the WG2 document was compiled. During subsequent meetings, this document has been added to, scrutinised and amended, and a final version was prepared for submission to the GAMA Group at the end of August 2004. Close liaison was always maintained with the other two CFD Writing Groups (items 1 and 3 above) to ensure a minimum of overlapping material, and that the content of the reports remained within context. For completeness, two-phase CFD items have been identified in the WG2 document, but in outline only, deferring all details to WG3.

Results

The group has concentrated on single-phase phenomena, considering that two-phase CFD is not yet of sufficient maturity for a useful assessment basis to be constructed and that identification of the development areas (the task of Writing Group 3) should be undertaken first. Within this limitation, an assessment had been made of the current capabilities of CFD codes to perform trustworthy numerical analyses of NRS-related issues. A list (23 entries) of problems for which CFD analysis is required, or is expected to result in positive benefits, has been compiled, and reviewed critically by the group. The list contains safety issues of relevance, broadly categorised into core, primary-circuit and containment phenomena, under normal and abnormal operating conditions, and during accident sequences. The list is as comprehensive as the group could assemble given the time and cost constraints upon it.

Recognising that CFD is already an established technology outside of the nuclear community, the group drew up a list of the existing assessment bases, and discussed their relevance to the application of CFD to NRS issues. It was found that the databases were principally of two types: those concerned with general aspects of trustworthiness of code predictions (ERCOFTAC, QNET-CFD, FLOWNET), and those which focussed on particular application areas (MARNET, NPARC, AIAA). It was concluded that application of CFD to NRS problems can benefit indirectly from these databases, and the continuing efforts to extend them, but that a comprehensive NRS-specific database would be a more useful concept. The various efforts to improve the quality and trust in the use of CFD for NRS applications by means of validation exercises, as summarised in a series of NEA/CSNI documents and articles from Jahestagung Kern-technik, point in the right direction, but need to be brought into a common assessment database.

The group then identified, from a modelling viewpoint, the gaps in the existing assessment databases, and discussed the methodology for establishing assessment matrices specific to NRS needs. From these discussions, proposals were formalised for assembling, maintaining and extending an NRS assessment database. Details of the proposals are given in the WG2 document.

Finally, the scheduling of the tasks to be undertaken by the Writing Group, the lead organisations and estimates of the manpower effort required, were compiled.

Conclusions and recommendations

The group's proposal to extend the existing assessment base has three components.

- To form a working group to extend and consolidate the existing WG2 document to act as a platform for a web-based NRS assessment database, regulated by an NEA webmaster.
- As an ongoing action, the newly formed group would look for suitable experiments that could form the basis of benchmarking exercises specifically tailored to NRS needs, and to keep in touch with future programmes that could yield suitable benchmarking material. The group would become the organisational unit for this exercise.
- To organise an International Workshop, with OECD/NEA sponsorship, to promote the availability and distribution of experimental data suitable for NRS benchmarking, and to monitor the current status of CFD validation exercises relevant to NRS issues. The Workshop will also cover two-phase aspects. Vattenfall and GRS (Garching) have offered to host Workshop. Depending on the success of the venture, organisation of further Workshops on a regular basis is envisaged.

Scheduling

The table below is an estimate of organisational responsibility, level of effort and schedule for the tasks to be carried out by the newly formed WG2. It is based on the present group structure, and is subject to changes resulting from any new structure of the group, including replacement and/or new participation.

TASK	Lead	Support	Effort#	Report to WG
Forming of Working Group	OECD/NEA		1 day	Jan. 2005
Revision of Existing Document	PSI	All	3 days	Jan. 2005
Identify Suitable Benchmarks				
Core and HXs	Halden	Vattenfall/JNES	10 days	Jan. 2006
Primary Circuit	GRS	FZR/CEA	10 days	Jan. 2006
Containment	CEA	GRS/PSI	10 days	Jan. 2006
Workshop	“Host”	All	70 days	Mar. 2005
Web-Site Enhancement	OECD/NEA	All	1 day	Sep. 2006
Evaluation of Workshop	PSI	All	15 days	Dec. 2006
Recommendations for the Future	PSI	PSU	2 days	Mar. 2007

Anticipated commitment over two years: five days/year/group-member

Beyond 2006, an amalgamation of WG1 and WG2, together with the NEA webmaster, is proposed to drive the activities further. Future activities would include: (1) forming a control group, combining WG1 and WG2; (2) organisation of benchmark exercises; (3) definition of problem-specific Best Practice Guidelines (BPGs); (4) website maintenance; (5) organisation of further Workshops.

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1. INTRODUCTION/BACKGROUND

Computational methods have supplemented scaled model experiments, and even prototypic tests, in the safety analysis of reactor systems for more than 25 years. During this time, very reliable system codes, such as RELAP-5, TRACE, CATHARE and ATHLET, have been formulated for analysis of primary circuit transients. Similar programs (such as SCDAP, MELCOR, GOTHIC, TONUS, ASTEC, MAAP, ICARE, COCOSYS/CPA) have also been written for containment and severe accident analyses.

The application of Computational Fluid Dynamics (CFD) methods to problems relating to Nuclear Reactor Safety (NRS) is less well developed, but is accelerating. The need arises, for example, because many traditional reactor system and containment codes are modelled as networks of 1-D or 0-D elements. It is evident, however, that the flow in components such as the upper and lower plena, downcomer and core of a reactor vessel is 3-D. Natural circulation, mixing and stratification in containments is also essentially 3-D in nature, and representing such complex flows by pseudo 1-D approximations may not just be oversimplified, but misleading, producing erroneous conclusions.

One of the reasons why the application of CFD methods in Nuclear Reactor Safety (NRS) has been slow to establish itself is that transient, two-phase events associated with accident analyses are extremely complex. Traditional approaches using system codes have been successful because a very large database of phasic exchange correlations has been built into them. The correlations have been formulated from essentially 1-D special-effects experiments, and their range of validity well scrutinised. Data on the exchange of mass, momentum and energy between phases for 3-D flows is very sparse in comparison. Thus, although 1-D formulations may restrict the use of system codes in simulations in which there is complex geometry, the physical models are well-established and reliable, provided they are used within their specified ranges of validity. The trend has therefore been to continue with such approaches, and live within their geometrical limitations.

For containment issues, lumped-parameter codes, such as COCOSYS or TONUS-0D, include models for system components, such as recombiners, sprays, sumps, etc., which enable realistic simulations of accident scenarios to be undertaken without excessive computational costs. To take into account such systems in a multi-dimensional (CFD) simulation remains a challenging task, and attempts to do this have only recently begun, and these in dedicated CFD codes such as GOTHIC, GASFLOW or TONUS-3D rather than in commercial, general-purpose CFD software.

The issue of the validity range of CFD codes for NRS applications has also to be addressed, and may explain why the application of CFD methods is not straightforward. In many cases, even for single-phase problems, nuclear thermal-hydraulic flows may lie outside the range of standard models and methods, especially in the case of long, evolving transient flows with strong heat transfer.

It appears then that we have, maybe temporarily, maybe longer term, a technology gap between codes with primitive geometric capabilities, ancient numerical methodologies, but sophisticated physical models, and CFD, for which geometric complexity is no real problem, but for which, at least for two-phase and containment applications, the physical models require considerable further development.

The present activity arises from the need to critically assess[#] where CFD methods may be used effectively in problems relating to Nuclear Reactor Safety, and to demonstrate that utilisation of such advanced numerical methods, with large computer overheads, is justified, because the use of simpler engineering tools or 1-D codes have proven to be inadequate.

[#] The word *assess*, as used here, is a synonym for appraise, evaluate or judge.

The rest of the document is organised as follows. The objectives of the activity, which have been updated slightly from those originally set out in the CAPS (GAMA 2002 7, Revision 0, October 2002), are summarised in Section 2. The main body of the document is contained in Section 3, which provides a list of NRS problems for which the need for CFD analysis has been recognised, and in most cases also actively pursued. A few references are provided for orientation, but are not intended to be comprehensive. Two-phase problems requiring CFD are also listed for completeness, but all details are deferred to WG3. Brief summaries of existing assessment databases (mostly non-nuclear) are given in Section 4, and from this information the gaps in the assessment bases, with now particular emphasis on NRS applications, are summarised in Section 5. The suggested methodology for extending the existing assessment bases, and building a more NRS-oriented database, are set out in Section 6, and a summary given in Section 7. Finally, scheduling of the proposed tasks under Section 6, and a glossary of the acronyms introduced, are provided as annexes.

2. OBJECTIVES OF THE WORK

The basic objective of the present activity is to provide documented evidence of the need to perform CFD simulations in NRS (concentrating on single-phase applications), and to assess the competence of the present generation of CFD codes to perform the tasks required of them. The fulfilling of this objective will involve multiple tasks, as evidenced by the titles of the succeeding chapters, but, in summary, the following items list the specifics:

- To provide a classification of NRS problems requiring CFD analysis
- To identify and catalogue existing CFD assessment bases
- To identify shortcomings in CFD approaches
- To define a strategy for extending the CFD assessment database, with an emphasis on NRS applications.

3. NRS PROBLEMS WHERE (SINGLE-PHASE) CFD ANALYSIS BRINGS REAL BENEFITS

Introduction

The focus here will be on the use of CFD techniques for single-phase problems relating to NRS. This is the traditional environment for most non-NRS CFD applications, and the one which has a firm basis in the commercial CFD area. NRS applications involving two-phase phenomena will be listed in this document for completeness, but full details are reserved for the WG3 document, which addresses the extensions necessary for CFD to handle such problems.

The classification of problems identified by the Group is summarised in Table 1, and then, under appropriate sub-headings, a short description of each issue is given, why CFD especially is needed to address it, what has been achieved, and what further progress needs to be made. There are also moves within the nuclear community to interface CFD codes with traditional system codes. Identification of the needs of this combined approach is also contained in Table 1, and then addressed more fully in the subsequent sub-sections.

With some overlaps, the entries are roughly grouped into problems concerning the reactor core, primary circuit and containment, consecutively.

Table 1**: NRS problems requiring CFD with/without coupling to system codes**

	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
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

DBA – Design Basis Accident; BDBA – Beyond Design Basis (or Severe) Accident; MCPR – Minimum Critical Power Ratio

3.1 Erosion, Corrosion and Deposition

Relevance of the phenomena as far as NRS is concerned
Corrosion of material surfaces may have an adverse effect on heat transfer, and oxide deposits may accrue in sensitive areas. Erosion of structural surfaces can lead to degradation in the material strength of the structures.

What the issue is
The secondary circuit of a PWR is essentially made of carbon steel and copper alloys. Corrosion produces oxides, which are transported to the SGs and give rise to deposits (e.g. on the tube support plate). There are two effects due to the presence of sludge in the SGs:

- effect on the efficiency of the SGs;
- corrosion of SGs (plate and tube degradation).

In the primary circuit, the chemistry is different, but corrosion phenomena are also encountered, particularly on the fuel claddings.

The oxide layers resulting from corrosion have altered properties compared to the initial construction material. If the layers are thin enough, the effect on the overall structural integrity is negligible. Such a thin oxide layer is in fact protecting the structural material from further degradation. However, in certain circumstances, the oxide layer may be eroded, due to a local increase of wall shear stress. This is typically occurring at places where there is a sudden change of flow direction, for example at a channel entrance or sudden area change. In such circumstances, the protective oxide layer may be continuously eroded, leading to substantial changes in structure integrity.

What the difficulty is and why CFD is needed
The prediction of the occurrence of such phenomena requires simulation at very small scales. It is important to understand and predict primary and secondary circuit corrosion occurrence as well as sludge deposition in order to control and limit their occurrence. System codes and component codes, which use either homogenisation or sub-channel analysis, cannot predict the highly localised phenomena associated with corrosion and deposition, and there is a need for a detailed flow field analysis, with focus on the wall shear stress prediction. (In the case of two-phase flow, it may require CFD extension to properly treat the two-phase boundary layer.) The rate of the erosion primarily depends on water chemistry (pH level, fluid oxygen content) and material properties, but it is also influenced by the following fluid-mechanics parameters:

- fluid local velocity;
- fluid local temperature;
- flow local quality.

These local parameters are geometry-dependent, and can only be predicted with a proper CFD model.

3.2 Core Instability in BWRs

This is a two-phase phenomenon, and is covered in detail in the WG3 document.

Orientation
Flow instabilities in BWRs can induce power surges, because of the strong coupling between void fraction and neutronics. The coupling results in a feedback system that under particular conditions can be unstable. In these conditions, the core experiences neutron power surges, with a frequency of the order of 0.5 Hz, eventually leading to a reactor scram.

The prediction of local or out-of-phase oscillations requires detailed 3D calculations, both for the kinetics and thermohydraulic parts. A very detailed representation of the core and of its surroundings is desirable in order to obtain more reliable predictions. This includes a detailed nodalisation of the lower and upper plena and recirculation flow path.

Many computer codes have been used to predict stability behaviour in a BWR, but most of the available codes are based on drift-flux formulations. It is desirable to assess the benefits that could be achieved using two-fluid models for the prediction of channel stability. Moreover, a greater effort should be spent on benchmarking available codes against experimental data of real plant behaviour.

3.3 Transition boiling in BWRs – determination of MCPR

This is a two-phase phenomenon, and is covered in detail in the WG3 document.

Orientation
A large-break, loss-of-coolant-accident (LBLOCA) remains the classical design-basis-accident (DBA), in the sense that the emergency core-cooling (ECC) system has to be designed to be able to reflood the core and prevent overheating of the fuel cladding. During reflooding, multi-dimensional flow patterns occur. Though the physical phenomena are complex, CFD has the potential of following the details of the flow, with the aim of reducing uncertainties in current predictions made on the basis of 1-D system codes and 0-D lumped-parameter codes.

BWRs TechSpec requires that during steady-state operation the MCPR (Minimum Critical Power Ratio) thermal limit is kept above the licensed safety value. The MCPR tends to be a limiting factor at high burnup conditions. The current trend to extend plant lifetime and increase the fuel cycle duration requires improvements to be made in the methods used in the licensing analysis to estimate this limit. The use of CFD codes could lead to a significant decrease in the present, conservative assumptions employed.

3.4 Recriticality in BWRs

This is a two-phase phenomenon, and is covered in detail in the WG3 document.

Orientation
In a BWR severe accident, the first materials to melt are the control rods. This is due to the low melting temperature for the mixture of boron carbide and stainless steel. The situation can lead to core recriticality and runaway overheating transients. The resultant molten material accumulates on top of the lower support plate of the core. Some of it re-solidifies, supporting an accumulating melt pool. The supporting layer eventually breaks, and melt pours into the lower plenum.

Coolant penetration into the core during reflooding is assumed to occur due to a melt-coolant interaction in the lower plenum. No integral code is capable of describing all the necessary phenomena.

3.5 Reflooding

This is a two-phase phenomenon, and is covered in detail in the WG3 document.

Orientation
A large-break, loss-of-coolant-accident (LBLOCA) remains the classical design-basis-accident (DBA), in the sense that the emergency core-cooling (ECC) system has to be designed to be able to reflood the core and prevent overheating of the fuel cladding. During reflooding, multi-dimensional flow patterns occur. Though the physical phenomena are complex, CFD has the potential of following the details of the flow, with the aim of reducing uncertainties in current predictions made on the basis of 1-D system codes and 0-D lumped-parameter codes.

3.6 Lower Plenum Debris Coolability and Melt Distribution

Relevance of the phenomenon as far as NRS is concerned
During a severe accident in a nuclear power plant, the integrity of the nuclear reactor core is lost, and it can relocate to the lower plenum and form a debris bed. If cooling of the debris bed is not sufficient to remove the generated decay heat, a melt-through of the reactor pressure vessel will occur.

What the issue is
Estimates of debris coolability and melt relocation are highly empirical, and dependant on the particular design solutions used in the nuclear power plants. However, what is common to all the scenarios is the necessity to halt accident progression, remove the decay heat from the debris bed, and prevent melt-through of the vessel.

What the difficulty is and why CFD is needed
The following key parameters have to be taken into account in proper modelling of cooling of a debris bed:

- flow driving force (gravitation, capillary forces);
- flow resistance for both laminar flow (small particle areas) and turbulent flow (large particle areas);
- dryout criteria;
- counter-current flow limitation (CCFL);
- multi-dimensional effects;
- transient behaviour.

What has been attempted and achieved/what needs to be done (recommendations)
Current approaches remain empirical, and correlations are used to predict the heat transfer rate between particles and the cooling water. The water penetration through the bed is highly dependent on the bed structure (non-uniform particle distributions) and simplified approaches can be applied. CFD can be used to improve the accuracy of predictions in non-uniform beds. In particular, three-dimensional models of flow in a porous material will give better estimates of the water penetration rates, and relaminarisation due to different grain sizes.

Ref. 1: T.N. Dinh, V.A. Bui, R.R. Nourgaliev, J.A. Green, B.R. Sehgal, *“Experimental and Analytical Study of Molten Jet Coolant Interactions: The Synthesis”*, Intern. J. Nuclear Engineering and Design, 189, 299-327 (1999).

3.7 Boron Dilution

Relevance of the phenomenon as far as NRS is concerned
Boron concentration aims at controlling the power and subcriticality for shutdown conditions. Mechanisms supposed to lead to boron diluted water are known (consequence of small break, SG leakage etc. (ee Ref. 1 for a review).

What the issue is
The safety problem concerns the possible transport to the core of a diluted slug of water, and the related power excursion.

What the difficulty is and why CFD is needed
The whole phenomenon modelling requires 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 to this problem concern the description of the transportation mechanisms to the core: (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. CFD features of the simulation are the transient behaviour of the flow, the geometrical complexity of the computational domain, and the requirement of the precise mixing properties of the flow.

What has been attempted and achieved/what needs to be done (recommendations)
Boron dilution has been considered within an International Standard Problem (ISP-43, based on a University of Maryland Thermalhydraulic Facility allowing the mixing of flows of different temperature within a reduced scale vessel model, see Ref. 2).

Another scaled ($1/5^{th}$) model (ROCOM, Forschungszentrum Rossendorf) of the German PWR KONVOI has been considered for several test scenarios related to boron dilution transients (steady state, transient and cavity-driven flows may be considered). Some related results have been published (Ref. 1).

A third test facility is the Vattenfall model, built at Vattenfall Utveckling, Älvkarleby in 1992. It is a 1:5 scale model of the 3-loop Westinghouse PWR at Ringhals. The model has been used for several studies, including CFD simulations. International cooperation has been within the EUBORA project, and now the on-going FLOWMIX-R project, both of them EU 5^{th} Framework programmes.

For these databases, successful CFD results have been claimed, and applications to existing reactors have also been reported.

A concerted action on Boron Dilution Experiments (EUBORA, 1998, 4^{th} EC program) gathered several European countries involved in CFD applications for such problems. Many facilities provided relevant data: the EDF Bora Bora facility, the Rosendorf ROCOM facility, the UPTF facility, the PSI Panda facility (see Ref. 5). The conclusion from the EUBORA project was that 3-D CFD does provide an effective tool for mixing calculations, though the code calculations, and the applied turbulent mixing models, have to be validated by experiments. The current status on assessment is deemed not to be complete, it was concluded. A large-scale test (scale 1:2 tentatively) was also suggested to provide confirmation data.

The ongoing EU-project FLOWMIX-R aims at describing relevant mixing phenomena in the PWR primary circuit. It includes a well-defined set of mixing experiments in several scaled facilities (Rossendorf, Vattenfall, Gidropress and Fortum) to provide data for CFD code validation. Calculations are performed for selected experiments using two commercial CFD codes (CFX, FLUENT). The applicability of various turbulence modelling techniques is being studied for both transient and steady-state flows. Best Practise Guidelines (BPGs) are being applied in these computations. Homepage for FLOWMIX-R is www.fz-rossendorf.de/FWS/FLOMIX.

Also, an OECD action has recently started concerning a coolant transient for the VVER-1000 (Ref. 3).

Questions regarding the relevance of a test facility, when compared to reactor functioning conditions, may concern: (i) Re numbers (lower for the test facility, see discussion in Ref. 4), and (ii) complexity of the lower plenum, which may be different and lead to different mixing properties. The first point is considered as non-crucial, the second one may depend on the reactor considered.

Ref. 1: T. Hoene, H.M. Prasser, U. Rohde, *"Numerical coolant mixing in comparison with experiments at the ROCOM test facility"*, in proceedings of the ANS Conference, USA, 2001.

Ref. 2: T. Hoene, *"Numerical simulation of ISP-43 test using CFX-4"*, in proceedings of the ANS-ASME conference, Penn State University, 2002.

Ref. 3: NEA/NSC/DOC(2003) document on OECD/DOE/CEA VVER-1000 Coolant Transient Benchmark – 1st Workshop.

Ref. 4: T. Hohne, *"Coolant mixing in pressurized Power Reactor"*, 1999, in Proceedings of ICONE 7.

Ref. 5: H. Tuomisto, *et al.*, *"EUBORA - Concerted Action on Boron Dilution Experiments"*, FISA-99 Symposium on EU Research on Severe Accidents, Luxembourg, 29 November - 1 December, 1999.

Ref. 6: ISP-43: Rapid Boron Dilution Transient Experiment, Comparison Report, NEA/CSNI/R(2000)22.

Ref. 7: B. Hemström, R. Karlsson, M. Henriksson. *"Experiments and Numerical Modelling of Rapid Boron Dilution Transients in a Westinghouse PWR"*. Annual Meeting on Nuclear Technology, Berlin, May 2003.

3.8 Mixing, Stratification, Hot-Leg Heterogeneities

In-vessel mixing phenomena

Relevance of the phenomenon as far as NRS is concerned

PWRs have two to four coolant loops, depending on the design. It is important for reactor control that cold water fed from these loops is thoroughly mixed before entering the core, otherwise the safe operation of the reactor could be compromised.

What the issue is

The issue is the study of the mixing phenomena occurring in the downcomer and lower plenum of the reactor in the case of an accidental transient leading to asymmetric loop-flow conditions in terms of temperature or boron concentration. Transients such as Main Steam Line Break, accidental or inherent dilution transients are relevant to this issue. In these scenarios, flow in one or more of the hot legs is colder or non-borated with respect to the other loops. In the case of poor mixing, cold or low borated water can be injected into the core leading to recriticality returns, with a risk of cladding failure and fuel dispersion.

In general, the simulation of these transients requires the coupling of systems codes, to represent the whole primary circuit, and a part of the secondary circuit except the core. Core inlet conditions (flowrates, temperature or enthalpy) are deduced from vessel inlet conditions by the application of a mixing matrix. Up to now, the coupling is weak and mainly external (close-ups, boundary conditions, etc.), but attempts are being made to have a stronger coupling (see, for example, the OCDE/CSNI PWR Main Steam Line Break Benchmark).

Description of the difficulties and why CFD is needed to solve it
Mixing in the downcomer and lower plenum, up to now, as far as we know, have been modelled using mixing matrices obtained by extrapolation of steady-state test results, and not always with the actual lower plenum geometry (i.e. including downcomer and lower plenum internal structures), and not always under real operating conditions (in general, a constant mixing matrix is used). These matrices are then introduced as input to system codes, or used as an interface between a system code and a 3D core thermal-hydraulic code.

The use of CFD codes for the real reactor case, validated against data from the tests that has led to the definition of the mixing matrix, would represent a big step forward, since CFD offers the possibility to deal with the detailed geometry of the reactor and, in the “near” future, with transient flow conditions.

In the short term, CFD calculations would help identify the mixing laws used in the actual schemes (systems codes, coupled system, 3D core thermal-hydraulic and neutronics codes) in use, and in the medium term, one could imagine integration of a CFD code into the coupled chain: i.e. system, CFD, core 3D thermal-hydraulic and neutronics codes operating together. Finally, in the long term, if the capability of CFD codes is assessed for core thermal-hydraulic simulation, one could imagine the use of CFD for lower plenum and the core, coupled to 3D neutronics codes.

State of the art - recommendations
In a first step, one could focus on the application of CFD independent of any coupling with other types of codes. Up to now, CFD has been applied with some encouraging results for steady-state calculations of mixing phenomena in plena with internal structures (see for example Hot Leg Heterogeneities, Section 3.8).

The mixing process of feedwater and reactor water in the downcomer of an internal-pump BWR (Forsmark 1 & 2) has been numerically modelled using the CFD code FLUENT/UNS. Earlier studies, with a very coarse model (Hemström et al., 1992), had shown that a new sparger design is necessary to achieve an effective HWC through improved mixing in the downcomer. This requires detailed and accurate modelling of the flow, not only for determining the mixing quality, but also for avoiding undesirable effects, such as increased thermal loading of internal parts.

A 90-degree sector model, as well as smaller sector models, was used. The 90-degree model covered one (of four) spargers, two main coolant pumps (of eight), and flow from the steam separators. Some results are presented in Ref. 2 below. No verification tests have so far been performed, but hydraulic model tests of 1:5 scale or larger have been suggested.

The main difficulty in the application of CFD codes to such problems is linked to the mesh resolution, and the capability to manage the simulation under acceptable conditions (very long CPU times are required) due to:

- the complexity and expanse of the geometry to be modelled: at least the four hot legs and junctions with the core vessel, the downcomer and the lower plenum, together with all their internal structures;
- the difficulty in building the mesh due to the quite different scales in the domain (from a few cms to several metres); and
- the need to perform transient calculations, with or without coupling to system codes and 3D core physics codes.

Consequently, application of CFD codes in such a field requires, mainly:

- validated models, especially models of turbulence, to estimate the mixing in the lower plenum,
- good capacity to treat complex geometries of very different sized scales.

A second step will be to treat all the difficulties related to the coupling of CFD codes with system codes, other 3D component codes, and with 3D neutronics (see Section 5.2).

Ref. 1: OCDE/NEA – US/NRC PWR Main Steam-Line Break Benchmark, http://www.nea.fr/html/science/egrsltb/pwrmslbb/index.html

Ref. 2: Tinoco, H. and Einarsson, T., "*Numerical Analysis of the Mixing and Recombination in the Downcomer of an Internal Pump BWR*", Modelling and Design in Fluid-Flow Machinery, 1997.

Hot Leg Heterogeneities

Relevance of the phenomenon as far as NRS is concerned
For the safe running and control of a PWR, it is essential to have, as precisely as possible, knowledge of the real primary flow rates, to ensure that they do not exceed the limiting design basis values.

Description of the issue
The issue refers to the estimation of the flow-rates in a PWR plant. Indeed, for safe running, the real primary flowrates in the loops and the core have to be checked to ensure they do not exceed the limiting design-basis values. The upper value is deduced from mechanical considerations regarding the assembly holding forces, and on the control rod falling time, the lower value is associated to the DNB risk protection signal.

The real primary flowrates are deduced from on-site periodic measurements.

For each loop, the flow-rate is determined from the following formula:

$$Q_{loop} = \frac{3.6 \times 10^{6}}{\rho_{CL}} \times \frac{W_{SG} - W_{RCP}}{H_{HL} - H_{CL}} \qquad /1/$$

with :

- W_{SG} : thermal power extracted from the SG, deduced from a heat balance on the SG secondary side,

- W_{RCP}: thermal power given by the Reactor Coolant Pump, obtained via the RCP power measurement,
- ρ_{CL} : water density, given by the water property determination,
- H_{HL} : Hot Leg enthalpy,
- H_{CL} : Cold Leg enthalpy.

These two enthalpies are deduced from temperature measurements of the Hot and Cold legs of the loop under consideration.

In order to check if the estimated value does not exceed the criterion, the uncertainty on the final value has to be estimated. This uncertainty is a combination of all the basic uncertainties resulting from the measurement devices, and to the methodology used to determine the different elements in Equation /1/.

By far the main source of uncertainty (about 10 times greater than the other sources) is related to the estimation of the hot-leg temperature. Two kinds of uncertainties are involved in this estimation:

1. the first (easy to estimate) is generated by the measurement-chain precision;
2. the second is due to a lack of representation of the three temperature measurement locations used to estimate the *average temperature in regard to the real average temperature*.

Concerning the second uncertainty, despite the mixing processes in the upper plenum, important temperature and flow heterogeneities are still present at the hot-leg instrumentation location, leading to uncertainties in the estimation of the real average temperature. Consequently, in order to quantify this error, the real average temperature of the hot-leg has to be estimated from specific experimental tests, from specific plant tests, and finally by calculation.

Description of the difficulties and why CFD is needed to solve it
Direct extrapolation of experimental results to the real plant is very difficult, and often leads to an overestimation of the uncertainty. The use of this overestimated value in the case of plant modifications *(e.g.* core loading,…), can give results which do not satisfy the safety criteria. Advanced methodologies based on CFD calculations are then required in order to reduce this overestimation.

State of the art - recommendations
The situation at present is that CFD calculations have shown encouraging results. They are able to reproduce qualitatively all the phenomena observed during the experiments: the upper-plenum flow, the temperature contours from the core to the hot legs, and the flow pattern in the hot legs, composed of two rotating counter-current vortices. Nevertheless, some discrepancies remain, such as the location of the centre of these vortices along the hot-leg pipe.

The main difficulties in the application of CFD codes for such a physical issue are listed below.

1. The complexity and the expanse of the geometry to be modelled – the upper part of the core, the upper plenum and the dome, with all their internal structures, and the hot leg – and the very different scales (from 1 cm to a metre) of all the structures, lead to very difficult meshing problems, and to very expensive computations (involving several millions of meshes).

2. There are complexities involved in specifying the boundary conditions (core outlets, inner flow-rates in the lead tubes,…), and difficulties in initialising the turbulence levels.

3. Very fine representation of the turbulent phenomena is required to localise the vortices in the hot leg. Consequently, application of CFD codes in such a field requires validated models, especially models of turbulence, to estimate mixing in the upper plenum and vortex development in the hot leg.

A good capacity to treat complex geometries, of very different scales, is also required.

3.9 Heterogeneous Flow Distributions

Steam generator tube vibration (fluid/structure interaction)

Relevance of the phenomenon as far as NRS is concerned
Vibrations of the steam generator tubes are due to hydraulic forces arising from the flow around the tube bends; these are fluid/structure interaction problem. The vibrations mainly concern the part of the generator where either cross-flows develop (as, for example, for the single-phase flow at the generator inlet) or two-phase flows take place (in the evaporation region). Excessive vibrations of the tubes can lead to tube rupture. If this occurs, there will be mixing of primary and secondary circuits, and a (nominal at least) breach of the primary containment barrier. Improved understanding of the phenomena can lead to improvements in geometry, and better inspection procedures.

What the issue is
Flow-induced vibration is significant at the U-bend section of the tubes, and anti-vibration bars are installed in some designs to restrict the amplitude of the vibration. A global understanding of the vibration excitation mechanism is proposed in Ref. 1, as well as a collection of reference data. Actual vibration modelling relies on estimation of excitation sources, hydrodynamic mass, damping phenomena, mean velocity, void fraction, etc., without the support of CFD. However, a better (assessed) prediction of such quantities may come from a finer flow description, and knowledge of local, small-scale quantities.

What the difficulty is and why CFD is needed to solve it
System codes, such as RELAP5, cannot model the flow-induced vibration, or the mechanical interaction between the fluid and the structure. The coupling of the fluid and structure calculations is generally difficult, since (at least for Lagrangian modelling approaches) the mesh structure for the fluid calculation may change due to the motion of the structure. The relevant description should provide realistic mean values for future vibration models, and local values for coupled fluid/structure modelling in regions of complex flow. Both single-phase and two-phase flows are involved. For the first, existing models may provide some details, even if suitable assessment is required. Two-phase flow solvers may not yet be considered mature enough to provide relevant information for such phenomena.

What has been attempted and achieved / What needs to be done (recommendations)
Some new experiments are proposed in Ref. 1, to complement those being conducted by CEA: for example, the Panachet experiment, which considers single-phase cross-flow over a matrix of tube bundles. Also noteworthy are the first attempts at simulation using a CFD tool. Fluid-structure interaction is not taken into account in many commercial CFD codes, though developments are now underway. Coupling of a reliable two-phase CFD code, if one exists, and a computational structural dynamics code is necessary to calculate the U-tube vibration, since the structural motion has a feed-back on the flow dynamics.

Ref. 1: *"Flow induced vibration: recent findings and open questions"*, Pettigrew, Taylor, Fisher, Yetisir, Smith, Nuclear Engineering and Design, 185, 249-276 (1998).

3.10 BWR/ABWR Lower Plenum Flow

Relevance of the phenomenon as far as NRS is concerned

There are many pipes in the lower plenum of a BWR or ABWR reactor. Two phenomena are relevant to NRS. One is the stress induced by flow vibration, which may cause these pipes to break, and the other is a lack of uniformity of flow between the pipes, which may lead to a non-uniform temperature distribution in the reactor core.

What the issue is

In an ABWR, the reactor internal pumps are newly installed at the side, near the base of the reactor pressure vessel. (Fig. 1, Section 3.22) The following two problems are to be solved.

(1) Many internal structures, such as guidance pipes of control rods and instrumentation pipes for neutron flux detection, are situated close together in the lower plenum. It is necessary to check the integrity of these structures against flow induced-vibration stresses(Fig.2, Section 3.22).

(2) In an ABWR, partial operation of the reactor internal pumps is accepted. However, it is necessary to check that the coolant is uniformly distributed to the reactor core during such operation.

What the difficulty is and why CFD is needed to solve it

Many internal structures are located close together in the lower plenum. At a time of partial pump operation, inverse flow can occur in the leg attached to the pump which has stopped. CFD codes are effective in evaluating the flow field in such complicated situations.

What has been attempted/achieved so far and what needs to be done.

The three-dimensional flow field in the reactor vessel has been evaluated successfully using the CFD code STAR-CD, with the standard k-epsilon turbulent model.

Ref. 1: S. Takahashi, *et al*., *"Evaluation of Flow Characteristics in the Lower Plenum of the ABWR by using CFD Analysis"*, ICONE-11, Tokyo, JAPAN, April 20-23, 2003.

3.11 Waterhammer Condensation

Relevance of the phenomenon as far as NRS is concerned

Fast closing (or even opening) of valves induces strong pressure waves, which propagate through the circuit, both in the primary and secondary loops. The dynamic effects on the pipework could induce damage, and are therefore a safety concern.

What the issues are

Waterhammer is most often investigated with respect to the mechanical loads applied to the pipe structure, resulting from pressure waves. This is connected to the study of ageing phenomena of nuclear pressure vessel materials.

What the difficulty is and why CFD is needed

The main issue concerns the loads applied to the structure. This implies knowledge of additional quantities, such as condensation speed, velocity and pressure distributions, from which depends the mechanical loading to the pipes. All these phenomena are characterised by very fast transients. The simulation typically requires very small time steps, and may be conducted using a one-dimensional code. Three-dimensional codes are required when volume effects are involved, for example in the hot leg.

The waterhammer phenomenon can develop along with stratification (thermal or phase induced), and this also has three-dimensional features: occurrence of radial pressure distributions [1] and three-dimensional turbulence effects. Code assessment needs to take care of the different possible geometries: straight pipes, elbows, change of pipe diameter, etc. The accurate evaluation of these quantities may require CFD.

What has been attempted and achieved/What needs to be done (recommendations)
Basic considerations for code assessment may be required for waves developing in liquids and gases: examples are air and water [2], and subcooled water and steam for vertical and/or horizontal pipes [3]. Available measurements would concern pressure at different positions in the pipes, and, in particular, in sensitive areas, such as the measurement of the condensed phase at the end of the pipe.

Results of the WAHALoads (Two-Phase Flow Water Hammer Transients and Loads Induced on Materials and Structures of Nuclear Power Plants) EC programme may be of interest in the near future. The WAHALoads group may select and open for public use a set of relevant experiments undertaken during the program. This should be done in the spirit of a benchmarking activity and related code assessment.

Ref. 1: http://www.fz-rossendorf.de/FWS/publikat/JB99/jb99_sum.pdf

Ref. 2: K. W. Brinckman, M. A. Chaiko, *"Assessment of TRAC-BF1 for waterhammer calculations with entrapped air"*, J. of Nuclear Technology, 133(1), 133-139 (2001).

Ref. 3: Gaddis and Harling, *"Estimation of peak pressure-rise in a piping system due to the condensation induced waterhammer phenomenon"*, Proceedings of ASME/JSME Fluid Engineering Division Summer Meeting, 1999.

3.12 Pressurised Thermal Shock (PTS)

Relevance of the phenomenon as far as NRS is concerned
PTS is related to the ageing of the vessel (because the mechanical resistance of the structure decreases with age). The events of concern are cold-water injections – which would, for example, accompanying a Loss of Coolant Accident followed by Emergency Core Cooling System (ECCS) injection; a Main Steam Line Break; a steam generator tube rupture; a small break loss of coolant; etc. (see Refs. 1 and 2) – that may lead to a thermal shock. Both single-phase and two-phase flow situations may occur.

What the issue is
The issue is to predict the temperature (and the related thermal stresses) for the part of the vessel subjected to thermal shock, in order to investigate thermal fatigue, and the mechanical stresses to the vessel. Limited to the CFD concerns, the temperature of the vessel is determined through the temperature of the water in contact with the walls, and is influenced by turbulence, stratification (for both single- and two-phase situations), and, in the case of two-phase flows, by the condensation rate (the issue is connected with the direct-contact-condensation issue). The CFD issues are to take into account these features for the whole transient (which may last for several hundreds of seconds), for complex geometries (downcomer, upper plenum, and connected pipes), and for complex flow patterns (stratified flows, jets, plume development in the downcomer, etc.).

What the difficulty is and why CFD is needed
The temperature of the vessel is determined through the temperature of the fluid in contact with it, and is influenced by turbulence (which enhances mixing), stratification (for both single- and two-phase situations), and by the condensation rate (for two-phase flow).

The whole phenomenon is unsteady, 3-D, and the precise determination of all the parameters is complex. The existing reported simulations concern single-phase flow, whereas simulations of two-phase flows in such situations are just beginning. Concerning single-phase flows, however, the precise description of the problem is reported to require turbulence models where both low Reynolds effects, laminar to turbulence transition and buoyancy effects need to be taken into account (Ref. 3).

What has been attempted and achieved/what needs to be done (recommendations)

No systematic assessment has yet been reported, and only the system codes may be considered as validated against this problem. Although the single-phase CFD applications seem mature enough to be used, reported attempts were not all successful (see Ref. 3), and the further use of relevant experimental data and turbulence modelling improvement has been suggested (see Ref. 5).

For CFD, two assessment methods may be considered. Firstly, an assessment has to be made of the ability of a method to reproduce a particular phenomenon within the whole transient: one may consider the capability of the method to solve unsteady, coupled problems between the structure and the flow (thermal fatigue issue), the ability to describe stratification, to estimate condensation for different flow patterns (reported uncertainties concern for example the Heat Transfer Coefficient (HTC) inside the plumes). Secondly, the assessment should take into account an entire thermal shock sequence with the complete geometry. Reported relevant experiments are:

COSI: the COSI experiment is scaled 1/100 for volume and power from a 900 MW PWR and allows various flow configurations. Simulations representing small break LOCA thermal-hydraulic conditions, and including temperature profiles at various axial positions in the pipe and condensation rates, are reported in Ref. 1.

An international study concerning PTS (International Case RPV PTS ICAS) has been completed, and proposed comparative assessment studies for which CFD codes could be used (Ref. 4). Reported data used for thermal-hydraulic tests concern the Upper Plenum Test Facility (UPTF) in Manheim. Particular attention was paid to thermal-hydraulic mixing. A first description of UPTF facility is available at the following web-site: http://asa2.jrc.it/stresa_framatome_anp/specific/uptf/uptffac.htm, or at http://www.nea.fr/abs/html/csni1004.html.

For both single- and two-phase flows, model improvement seems to be required. (See also the requirements for two-phase flows models in the work of the writing group on two-phase flow CFD.)

Ref. 1: P. Coste, *"An approach of multidimensional condensation modelling for ECC injection"*, in the Proceedings of the European Two Phase Flow Group Meeting, 2003.

Ref. 2: H.K. Joum, T.E. Jin, *"Plant specific pressurized thermal shock evaluation for reactor pressure vessel of a Korean nuclear power plant"*, in the Proceedings of the International Conference on Nuclear Energy in Central Europe, 2000.

Ref. 3: J. Sievers, HG Sonnenburg, *"Modelling of Thermal Hydraulic Loads and Mechanical Stresses on Reactor Pressure Vessel"*, presented at Eurosafe 1999.

Ref. 4: *"Comparison report of RPV pressurized thermal shock international comparative assessment study (PTS ICAS)"*, 1999, NEA/CSNI/R(99)3 report.

Ref. 5: *"Advanced Thermohydraulic and neutronics codes: current and future applications"*, 2001, NEA/CSNI/R(2001)1/VOL1 report.

3.13 Pipe Break

Relevance of the phenomenon as far as NRS is concerned
Transient pressure forces occur on the structures following a large pipe break, and are of importance for various reactors. Inside the reactor vessel, the decompression waves will produce dynamic loadings on the surfaces of the vessel internals, such as the core shroud and core grids of a BWR.

What the issue is
This issue is an important example of the need to predict accurately three-dimensional, transient pressure fields, in order to estimate dynamic loadings on the internals. Structural analysis nowadays has to include dynamic loads, even for loss-of-coolant accidents.

What the difficulty is and why CFD is needed
The decompression process is a highly three-dimensional and transient phenomenon, so it is well suited for a 3D CFD simulation. During the first phase, before flashing of the reactor water begins, a single-phase CFD model could be used. After flashing has started, a two-phase model is necessary to describe the decompression process, since then two-phase effects are dominant.

What has been attempted and achieved/what needs to be done (recommendations)
CFD analysis of a steam line break in a BWR plant was part of a qualifying programme before the replacement of core grids at Units 1 and 2 at Forsmark NPP, Sweden, [Ref. 1]. The study was based on the assumption that the time scale of the transient analysis is smaller than the relaxation time of the water-steam system.

The results displayed a rather complex behaviour of the decompression, and the instantaneous forces computed were approximately twice those estimated in the past using simpler methods. It was pointed out that, at longer times, a two-phase model is necessary to describe the decompression. The results have not been validated against experiments, however.

During the last few years, several other simulations of rapid pipe breaks have been performed for Swedish reactors, also with no possibilities to compare with experimental results. Validation against HDR Experiments was therefore foreseen. In the early 1980s, the HDR (Heissdampfreaktor) blow-down experiments had been performed in Karlsruhe, Germany [Refs. 2 and 3]. The HDR rig consists of a blow-down nozzle, and a large pressure vessel, including internals (core barrel). The blow-down experiment V31.1 has been used for validation of numerical simulations, first using system codes, such as RELAP [e.g. Ref. 4], and later also with CFD (or CFD-like) codes. Lars Andersson et al. [Ref. 5] has presented simulation results using Adina-FSI (a coupling between the codes Adina-F (CFD) and the Adina structure solver) at the ASME PVP 2002 conference. The conclusions were that the results based on a single-phase fluid model, with no possibility of phase change, and with fluid-structure-interaction (FSI), compare well with experimental data for the first 100 ms after the break. Without FSI, the simulations show a factor 2 higher frequency for the pressure oscillations, and the amplitudes were generally higher. The conclusion was that the effects of FSI have to be included to obtain reliable results.

Ref. 1: Tinoco, H., *“Three-Dimensional Modelling of a Steam-Line Break in a Boiling Water Reactor”*, Nuclear and Engineering, 140, 152-164 (2002).

Ref. 2: Wolf, L., *“Experimental results of coupled fluid-structure interaction during blow down of the HDR-vessel and comparison with pre- and post-test prediction”*, Nuclear Engineering and Design, 70, pp. 269-308 (1982).

Ref. 3: HDR Sicherheitsprogramm. Auswertung von Dehnungsmessungen am HDR-Kernmantel und vergleich mit Spannungsberechnungen bei Bruch einer Reaktorkühlmittelleitung. Auswertebericht Versuchsgruppe RDB-E II. Versuche: V31.2, V32, V33, V34.

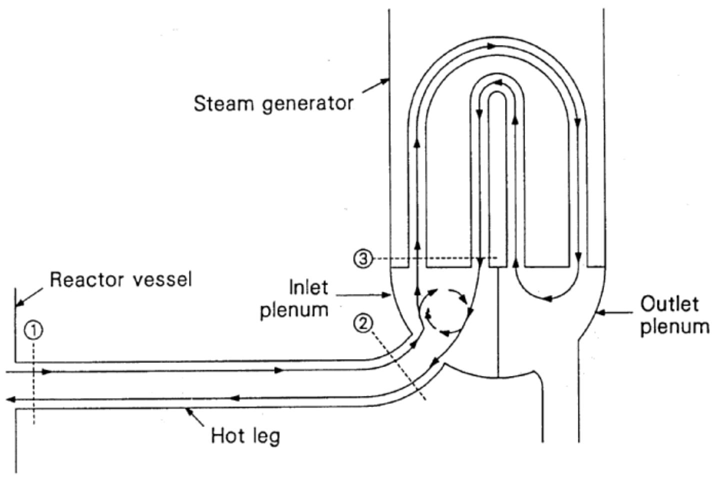
Ref. 4: Müller, F. Romas, A., ”Validation of RELAP-5 against HDR-experiments”, DNV-Kärnteknik, 2002.

Ref. 5: Andersson, L., Andersson, P., Lundwall, J., Sundqvist, J., Veber, P., “Numerical Simulation of the HDR Blowdown Experiment V31.1 at Karlsruhe”, PVP-Vol. 435, Thermal-Hydraulic Problems, Sloshing Phenomena and Extreme Loads on Structures, ASME 2002.

3.14 Induced Break

Relevance of the phenomenon as far as NRS is concerned
This scenario is of direct safety relevance because it involves core uncovery, and could lead to rupture of the primary circuit due to thermal loading.

Description of the issue
This subject is devoted to PWR induced break during a high pressure severe accident (for example: due to station blackout or loss of secondary feed water). In this kind of scenario, the core is uncovered, heat is carried away from the fuel by steam in a process of natural circulation to structures in the reactor coolant system, including the upper vessel, hot leg, and steam generator tubes. In these scenarios, the loop seals are filled with water and full primary loop circulation is blocked. A counter current natural circulation pattern in the hot leg and steam generator (with direct and reverse circulation in different SG tubes) is predicted, and experimentally observed.



The scenario ultimately leads to a failure due to thermo-mechanical loads in the primary coolant loop. The flow field and heat transfer details determine whether the failure occurs within the containment, in the reactor coolant piping system, in the reactor vessel, or in the steam generator tubing with a leak path out of containment.

The flow and heat transfer phenomena govern the temperature of the steam in the pipes, in the steam generator inlet plenum, and in the tubes. In order to determine if the tubes remain intact during this type of accident, mechanical studies should be made on each component likely to break. Therefore, the thermo-mechanical loads have to be estimated.

The key parameters addressed in these evaluations are the mixing within the steam generator inlet plenum (hot steam coming from the core and "cold" steam from the reverse flow in the SG tubes), the intensity of the thermal stratification in the hot leg, and the quantification of direct and reverse flow in SG tubes.

Description of the difficulties and why CFD is needed to resolve them

The thermal-hydraulic and core-degradation modelling of this severe accident scenario is performed using lumped parameter codes such as SCDAP/RELAP5, CATHARE/ICARE, etc. The efficiency of the lumped parameter approach makes it feasible to predict the transient behaviour of the entire reactor coolant system over extended periods of time. The limitations of this approach are the reliance on pre-determined flow paths and flow-split ratios that are used to adjust the inlet plenum mixing to pre-defined values, and the proportion of direct and reverse SG tubes.

Another difficulty is the extrapolation of these results in terms of the 3D thermal loads needed for the mechanical studies, due to the fact that the specifics of the geometry cannot be taken into account in these calculations (elbows, non-symmetry of the entrance of the hot leg in the inlet plenum, etc.).

For these reasons, and also because of a lack of experiments under reactor conditions, CFD calculations are required in parallel to the lumped-parameter approach in order to:

- adjust the models used in lumped-parameter codes (inlet plenum mixing, partition between direct and reverse SG tubes…);
- define more precisely the (3D) thermal loads on the different structures of the circuit;
- validate as far as possible the results from the lumped-parameter calculations.

State of the art - recommendations

Up to now, CFD has been applied with some encouraging results for steady-state calculations of the reactor case [1,2] and for one experimental validation case [3]. The main difficulties in the application of CFD codes for such an accident are:

- the complexity and expanse of the geometry to be modelled: at least one hot leg with the pressuriser surge line, the primary side of the steam generator, including both plena (inlet and outlet) and the SG tubes – this degree of detail causes many meshing problems;
- the necessity to represent more accurately the heat exchange with the different structures and so to accurately reproduce the thermal behaviour of these structures;
- the level of temperature, which often necessitates to take into account the exchanges by radiation between the fluid (hot and cold parts of it) and the structures;
- the nature and properties of the fluid (a mix of steam and hydrogen, in variable proportions).

Consequently, application of CFD codes in such a field requires:

- validated models, especially models of turbulence, to estimate mixing and stratification;
- a validated model of radiative exchange (with steam and hydrogen at high temperatures);

- simplified, but accurate, nodalisation of the tube bundle (inlet flow) – the solutions one can imagine are to couple 1D and 3D models, or to define some equivalent, in order to reduce the size of the mesh;

- validated models of the depressurisation induced by the opening of the safety valves (compressible or quasi-compressible model).

Ref. 1: H. Mutelle, U. Bieder *"Study with the CFD Code TRIO_U of Natural Gas Convection for PWR Severe Accidents"*, NEA and IAEA Workshop: Use of computational fluid dynamics (CFD) codes for safety analysis of reactor systems including containment - PISA ,Italy, November 11-15, 2002.

Ref. 2: U. Bieder, C. Calvi, H. Mutelle *"Detailed thermal hydraulic analysis of induced break severe accidents using the massively parallel CFD code TRIO_U/PRICELES"*, SNA 2003 International conference on super computing in nuclear applications, Paris, France, 22-24 Sept. 2003.

Ref. 3: C. Boyd and K. Hardesty, *"CFD Predictions of Severe Accident Steam Generator Flows in a 1/7th Scale Pressurized Water Reactor"*, Tenth International Conference on Nuclear Engineering, ICONE-10, April 14-18 2002, Arlington, Virginia.

3.15 Thermal Fatigue in Stratified Flows

Relevance of the phenomenon as far as NRS is concerned
Thermal stratification, cycling and striping phenomena may occur in piping systems in nuclear plants. They can occur in safety-related lines such as the pressuriser surge line, the emergency core cooling injection lines, and other lines where hot and cold fluids may come into contact.

What the issue is
Often the phenomena are caused by defective valves through which hot (or cold) water leaks into cold (or hot) water. Damage due to thermal loadings has been reported in mixing tees of the feedwater systems, in reactor clean-up systems, and in the residual-heat removal systems. Static mixers have been developed and used, since the first inspections indicated cracks. Thus, in general, the common thermal fatigue issues are understood and can be controlled. However, some incidents indicate that certain information on the loading in the mixing zone, and its impact on the structure, is still missing.

Under accident conditions, plume and stripe cooling in the downcomer may occur. Different flow patterns are present, depending on the flow rates in the ECC injection nozzles, and the downcomer water levels.

Two-phase flow may occur when cold water is heated through an isolation device by hot water, causing the cold water on the other side to rise above the saturation temperature. One may encounter stratified flows, low velocities, and sometimes the presence of air due to degassing. There might be low frequency flow fluctuations associated with temperature fluctuations, which may lead to thermal fatigue.

What the difficulty is and why CFD is needed to solve it
CFD is able to predict thermal loading of metallic structures. Single-phase CFD may need to include LES (Large Eddy Simulation) turbulence modelling, to be able to predict the frequency and amplitude of the large-scale fluctuations.

What has been attempted and achieved/what needs to be done (recommendations)
Current studies are focussed on single-phase situations. Development of a two-phase CFD code able to handle stratified flows with temperature and density stratification effects, with turbulent mixing effects, and possibly using LES for the liquid, would be useful for some two-phase situations.

Ref. 1: T. Muramatu *et al*., *"Validation of Fast Reactor Thermomechanical and Thermohydraulic Codes"*, Final report of a coordinated research project 1996-1999, IAEA-TECDOC-1318, 2002.

Ref. 2: T. Muramatu, *"Numerical analysis of non-stationary thermal response characteristics for a fluid-structure interaction system"*, Journal of Pressure Vessel Technology, Vol. 121, pp.276, 1999.

3.16 Hydrogen Distribution

Relevance of the phenomenon as far as NRS is concerned
During the course of a severe accident in a water-cooled reactor, large quantities of hydrogen could accumulate in the containment.

What the issue is
Detailed knowledge of containment thermal hydraulics is necessary to ensure the effectiveness of hydrogen mitigation methods. Condensation and evaporation on walls, pool surfaces and condensers needs to be adequately modelled, because the related mass and heat transfer strongly influence the pressure and mixture composition in the containment. The transient pressure rise causes certain explosion hatches to open (which defines the scenario). In addition, there is pressure loading to the structures. The mixture composition is very important, because it strongly determines the burning mode of hydrogen and the operation of the PARs (Passive Autocatalytic Recombiners).

What the difficulty is and why CFD is needed
Containments have very large volumes and multi-compartments. The situation occurring in the context of a severe accident is also physically complex. A too coarse nodalisation will not only lose resolution, but will smear the temperature and velocity gradients through numerical diffusion. Temporal discretisation is also an important issue, as accident transients must be simulated over several hours, or even days, of physical time. From a physical point of view, the flow model must also take into account condensation (in the bulk or at the wall), together with heat transfer to the structures. Condensation models are not standard in CFD codes.

An additional, and significant, difficulty in the application of CFD to hydrogen distribution problems relates to the way in which reactor systems, such as recombiners, spray systems, sumps, etc., are taken into account. CFD simulations without such system/component models will not be representative of realistic accident scenarios in nuclear reactor containments.

What has been attempted and achieved/what needs to be done (recommendations)
A State-of-the-Art report on this issue was proposed to the CSNI in 1995, and a group of experts convened to produce the document, which appeared finally in 1999. The twin objectives of the SOAR were to assess current capabilities to predict hydrogen distributions in containments under severe accident conditions, and to draw conclusions on the relative merits of the various predictive methods (lumped-parameter approaches, field codes, CFD). The report concentrates on the traditional containment codes (e.g. CONTAIN and GOTHIC), but acknowledges the future role of CFD-type approaches (e.g. GASFLOW, TONUS and CFX) to reduce numerical diffusion.

It was concluded that current lumped-parameter models are able to make relevant predictions of the pressure history of the containment and its average steam content, and that predictions of hydrogen distributions are adequate provided safety margins are kept high enough to preclude significant accumulations of sensitive mixtures, but that gas distribution predictions needed to serve as a basis for combustion analyses required higher resolution. The limits of the lumped-parameter approach have been demonstrated in a number of ISP exercises (notably ISP-23, ISP-29, ISP-35, ISP-37). CFD-type approaches may be the better option for the future, but considerable validation and accumulation of experience were considered necessary before such tools could be reliably used for plant analyses. An on-going benchmark exercise, ISP-47, aims precisely at validating CFD codes for containment thermal-hydraulics, including hydrogen risk.

Ref. 1: SOAR on Containment Thermalhydraulics and Hydrogen Distribution, NEA/CSNI/R(1999)16.

Ref. 2: A. Beccantini *et al*., *"H2 release and combustion in large-scale geometries: models and methods"*, Proc. Supercomputing for Nuclear Applications, SNA 2003, Paris, France, 22-24 September 2003.

Ref. 3: L. Blumenfeld et al., *"CFD simulation of mixed convection and condensation in a reactor containment: the MICOCO benchmark"*, Proc. 10th Int. Topical Meeting on Nuclear Thermal-Hydraulics, NURETH-10, Seoul, Korea, 5-9 October 2003.

3.17 Chemical Reactions/Combustion/Detonation

Relevance of the phenomenon as far as NRS is concerned
Detonation and combustion in containments may lead to pressure rises which exceed the design specifications. There is also risk of localised overheating of structures in the case of standing flames.

What the issue is
Although BWR containments are normally nitrogen inerted, which prevents hydrogen combustion and detonation, special attention has been addressed in recent years to possible leakage of hydrogen from the small overpressurised BWR containment to the reactor building, resulting in possible combustion and detonation, and providing a challenge for the containment integrity from outside.

For PWR containments that are not inerted, but which have some mitigation systems (recombiners, for example), local hydrogen concentrations can exceed the flammability limits, at least during some stages of the accident scenarios. Deflagrations, accelerated flames or even detonations are to be envisaged for some accident scenarios.

What the difficulty is and why CFD is needed to solve it
Deflagrations are very complex phenomena, involving chemistry and turbulence. No adequate models exist to accurately describe deflagrations at large-scale and in complex geometries – but still, CFD combined with flame-speed-based deflagration models can provide significant insight into the dynamic loadings on the structures.

Detonation processes are relatively simple to model, because the very fast front propagation means there is little feed-back from other, slower processes, such as chemistry, fluid flow and structural deformation. The interaction with the flow is limited to shock wave propagation – no turbulence models are necessary; in fact, it is generally sufficient to use the inviscid Euler equations. However, a fully compressible method must be used, typically a Riemann-type solver. Shock-wave simulations should account also for multiple reflections and superposition of the shock waves.

What has been attempted/achieved so far and what needs to be done

A project has been carried out under NKS/SOS-2.3 for the calculation of containment loads (BWR) in the above postulated scenario. The CFD code FLUENT was used to calculate hydrogen distribution in the reactor building, DET3D (Karlsruhe) for the 3D detonation simulation, and ABAQUS for the structural analysis and evaluation of the loads. The conclusion of this study was that a more detailed analysis would be required to take into account the pressure decrease after the detonation.

There have been many applications of compressible CFD solvers to model detonations in large-scale geometries (e.g. the RUT experiments from the Kurchatov Institute), and also some calculations of fast deflagrations in a simplified reactor containment (EPR) were performed in the framework of the 5th FP Project HYCOM. H2 deflagration models and CFD codes were also evaluated in the 4th FP project HDC (Hydrogen Distribution and Combustion).

Ref. 1: NKS-61 Advances in Operational Safety and Severe Accident Research, VTT Automation, Finland, 2002.

Ref. 2: A. Beccantini, H. Paillère, *"Modeling of hydrogen detonation for application to reactor safety"*, Proc. ICONE-6, San Diego, USA, 1998.

Ref. 3: U. Bielert *et al*., *"Multi-dimensional simulation of hydrogen distribution and turbulent combustion in severe accidents"*, *Nuclear Engineering and Design*, 209, 165-172 (2001).

Ref. 4: W. Scholtyssek *et al*., *"Integral Large Scale Experiments on Hydrogen Combustion for Severe Accident Code Validation"*, Final Report of HYCOM Project, Project FIKS-CT-1999-00004, to appear 2004.

Ref. 5: P. Pailhories, A. Beccantini, *"Use of a Finite Volume scheme for the simulation of hydrogen explosions"*, Technical meeting on use of CFD for safety analysis of reactor systems, including containment, Pisa, Italy, November 11-15, 2002.

3.18 Aerosol Deposition/Atmospheric Transport (Source Term)

Aerosol Deposition

Relevance of the phenomenon as far as NRS is concerned

Following a severe reactor accident, fission products would be released into the containment in the form of aerosols. If there were a subsequent leak in the containment barrier, aerosols would be released into the environment and pose a health hazard.

What the issue is

The most conservative assumption is that all the fission-product aerosols eventually reach the environment. A more realistic assessment can be made by studying the detailed processes which govern the initial core degradation, fission product release, aerosol-borne transport and retention in the coolant circuitry, and the aerosol dynamics and chemical behaviour in the containment.

What the difficulty is and why CFD is needed

The global thermal-hydraulic response is primarily determined by the balance of flow of steam from the circuit and condensation. The overall behaviour is therefore governed by the thermodynamic state, and is well reproduced using simple lumped-parameter models with coarse nodalisation (one or two volumes), provided the boundary conditions are correctly imposed. Nonetheless, it should be realised that the adequacy of simple representations perhaps depends on simple geometry and well-defined conditions. Care should be taken when extrapolating such conclusions to the much more complex situations encountered in a real plant.

Consequently, the controlling phenomena for aerosol removal need to be assessed using a more rigorous treatment of the forces acting on the particles. To simulate particle motion, it is necessary to know the 3-D velocity field, and CFD is needed for this purpose. The goal is to determine the accuracy with which CFD tools are able to predict the lifetimes of aerosols circulating in a large volume, such as a real reactor containment. By tracking a number of such particles, statistical information on the actual deposition can be obtained, and from that a realistic estimate of release in the event of a containment breach.

What has been attempted and achieved/what needs to be done (recommendations)
The PHEBEN-2 EU 5th Framework Programme aimed at improving the current analytical capability of realistically estimating power plant safety in the event of a hypothetical accident, based on the experimental information coming from PHEBUS-FP project. The PHEBUS-FP facility is operated at CEA Cadarache, and aims to investigate the key phenomena occurring in an LWR severe accident. The facility provides prototypic reactor conditions from which integral data on core degradation, fission product release, aerosol-borne transport and retention in the coolant circuit, and the aerosol dynamics and chemical behaviour in the containment may be obtained. The current programme comprises a series of five experiments, being carried out during the period 1993-2004, which simulate release and fission product behaviour for various plant states and accident situations. To date, four of the experiments have been performed; the final experiment in the present series is scheduled for 2004.

The experimental results from the PHEBUS tests performed so far confirm the appropriateness of lumped-parameter, coarse-node models for calculating the global response of the containment, at least for the simple geometry and conditions considered in the tests. There is no indication that detailed models or CFD methods are needed to calculate the global behaviour, though such methods are being applied to scope the potential. In any event, such approaches would be necessary to calculate the hydrogen distribution.

Ref. 1: P. von der Hardt, A.V. Jones, C. Lecomte., A. Tattegrain, *"The PHEBUS FP Severe Accident Experimental Programme", Nuclear Safety,* 35(2), 187-205 (1994).

Ref. 2: A. V. Jones *et al*., *"Validation of severe accident codes against PHEBUS-FP for plant applications (PHEBEN-2)"*. FISA-2001 EU Research in Reactor Safety, Luxembourg, 12-14 November 2001.

Ref. 3: A. Dehbi, *"Tracking of aerosol particles in large volumes with the help of CFD"*, Proceedings of 12th International Conference on Nuclear Engineering (ICONE 12), Paper ICONE12-49552, Arlington, VA, April 25-29, 2004.

Atmospheric Transport (Source Term)

Relevance of the phenomenon as far as NRS is concerned
During a severe reactor accident, radioactive release to the atmosphere could occur, which may represent a health hazard for the installation workers and the surrounding population.

What the issue is
Atmospheric release of nuclear materials (aerosols and gases) implies air contamination: on-site at first, and off-site with time. The atmospheric dispersion of such material in complex situations, such as the case of buildings in close proximity, is a difficult problem, but important for the safety of the people living and working in such areas. Dispersion models need meteorological fields as input; typical examples of such fields are velocity fields and characterisation of atmospheric thermal stability.

What the difficulty is and why CFD is needed to solve it
CFD provides a method to build and run models that can simulate atmospheric dispersion in geometrically complex situations; however, the accuracy of the results needs to be assessed. Emergency situations, which

lead to atmospheric release generally, involve two basic scales: on-site scale, where the influence of nearby buildings and source modelling are important phenomenon, and off-site scale (from a few kilometres to tens of kilometres), where specific atmospheric motions are predominant.

On-site atmospheric flows and dispersion are highly 3D, turbulent and unsteady, and CFD is a traditional approach to investigate such situations. Numerical modelling of building effects on the wind and dispersion pose several challenges. Firstly, computation of the flows around buildings requires knowledge of the characteristics of atmospheric boundary layers. In addition, knowledge of the mean wind speed and degree of atmospheric turbulence are also needed to accurately represent atmospheric winds, and the effects of the site, on dispersion. Secondly, topography of the configuration to be modelled is usually complex, especially in a Nuclear Power Plant, where closely spaced groups of buildings are commonplace, with different individual topologies, heights and orientations. Consequently, great challenges are encountered when discretising the computational domain. Thirdly, the flows are highly complex, having all the elements that modern fluid mechanics has not yet successfully resolved. The major challenge lies in turbulence modelling. The difficulty is associated with the fact that the flows are highly three-dimensional, being accompanied, almost without exception, by strong streamline curvature, separation, and vortices of various origin and unsteadiness.

What has been attempted/achieved so far and what needs to be done

While most of the CFD applications to date have been focussed on the generation of wind fields, as input to dispersion models for the purposes of assessment or emergency preparedness, the utilisation of prognostic models in weather-related emergencies is beginning to be explored. Prognostic model forecasting on regional scales will play an important role in advising local agencies regarding emergency planning in cases of severe accidents. In addition, model output information, such as precipitation, moisture and temperature, are often necessary for predicting the movement of pollutants under complex meteorological conditions. For example, wet scavenging during precipitation is an important sink of airborne pollutants leading to the deposition of contaminants.

Workstation-based meso-scale models have recently been used to provide real-time forecasts at regional scales, for emergency response to locally-induced severe accidents. In regional response forecasting, meteorological forecasts of 3-48h are generated continuously, with nested grid resolutions of 1-20 km, centred at the specific site of interest. These locally-generated forecasts are available for dispersion calculations.

Ref. 1: Fast J.D., O'Steen B.L., Addis R.P. *"Advanced atmospheric modelling for emergency response"*, *J. Applied Meteor*., 94, 626-649 (1995).

Ref. 2: Byrne C.E.I., Holdo A.E. *"Effects of increased geometric complexity on the comparison between computational and experimental simulations"*, J. of Wind Eng. and Indus. Aerodyn., 73, 159-179 (1997).

Ref. 3: Ding F., Arya S.P., Lin Y.L. *"Large eddy simulations of the atmospheric boundary layer using a new subgrid-scale model"*, Environmental Fluid Mechanics, 1, 29-47 (2001).

3.19 Direct-Contact Condensation

This is a two-phase phenomenon, and is covered in detail in the WG3 document.

Orientation
Some reactor designs feature steam discharge to cold-water pools. It is important to avoid steam by-pass in which vented steam may enter the vapour space above the pool and over-pressurise the confinement. The efficiency of the condensation process, and thermal mixing in the pool, may require detailed 3-D modelling using CFD.

3.20 Bubble Dynamics in Suppression Pools

This is a two-phase phenomenon, and is covered in detail in the WG3 document.

Orientation
Again, and related to direct contact condensation, it is important to avoid steam by-pass into the vapour space to avoid over-pressurisation. For some advanced passive cooling system designs, containment gases are vented to suppression pools. Even with complete steam condensation, bubbles containing non-condensable gases remain, and to assess their ability to mix the water in the pool, and avoid stratification, requires detailed CFD modelling.

3.21 Behaviour of Gas/Liquid Interfaces

This is a two-phase phenomenon, and is covered in detail in the WG3 document.

Orientation
In the two-fluid approach to two-phase flow modelling, as commonly employed in 1-D system codes and 3-D CFD codes, the two phases are treated as interpenetrating media. There are many instances of relevance to NRS in which the phases are physically separated and the phase boundary between them requires detailed resolution. Some examples are pressurised thermal shock (leading to thermal striping and cyclic-fatigue in structures), level detection in pressurisers, accumulators and the cores of BWRs (used for triggering ECC devices),and level swell in suppression pools. Given the 3-D nature of the flow regime, CFD methods, with direct interface-tracking capability, may be needed to accurately describe events.

3.22 Special Considerations for Advanced Reactors

Coolability of radial reflector of APWR

Relevance of the phenomenon as far as NRS is concerned
Insufficient cooling of the radial reflector causes thermal deformation of the reflector blocks, which results in formation of a gap between blocks. A leak flow through the gap decreases the core flow rate, and may raise the temperature of the reactor core.

What the issue is
The radial reflector consists of a stack of eight SUS304 blocks, in which many holes are installed to cool the reflector blocks, which become hot due to the heat generation of gamma rays. A large amount of the coolant which enters in the reactor vessel from the inlet nozzles flows up into the core region, and a small part of that flows into the radial reflector (Figs. 1,2) If the coolant flow rate into the radial reflector falls short, or becomes uneven circumferentially, the temperature of the coolant rises and the coolant may possibly boil.(Fig.3)

Since the reflector block is not symmetrical and the heat generation of gamma rays is not spatially uniform, the temperature distribution of the reflector block becomes uneven, and a deformation of the block due to the differences of the thermal expansion, produces a gap between the adjacent blocks. Consequently, the gaps cause bypass flow through from the reactor core side into the neutron reflector.

What the difficulty is and why CFD is needed to solve it
Evaluation of the temperature distribution in the reflector blocks with sufficient accuracy needs a detailed description of the coolant flow rate into the reflector. The details of this flow depend on the coolant flow field in the reactor vessel, and the flow field in lower plenum is complicated because of the asymmetrical arrangement of the structures. CFD is therefore the only effective tool for evaluating the coolant flow field in the reactor vessel.

What has been attempted/achieved so far and what needs to be done
The three-dimensional flow field in the reactor vessel, and the distribution of the coolant flow rate into the radial reflector, have been evaluated using the CFD code uFLOW/INS with the standard k-epsilon turbulent model. The uFLOW/INS code has been validated against experimental data from a 1/5-scale APWR experiment. Evaluation of the coolability of the radial reflector needs the correct calculation of the flow rates through the very small cooling holes installed in the reflector blocks. A technique is required for modelling these small holes without substantially increasing the total number of grid points used for the calculational domain.

Ref. 1: F. Kasahara, S. Nakura, T. Morii, and Y. Nakadai, *"Improvement of hydraulic flow analysis code for APWR reactor internals"*, CFD Meeting in Aix en Provence, May 15-6, 2002.

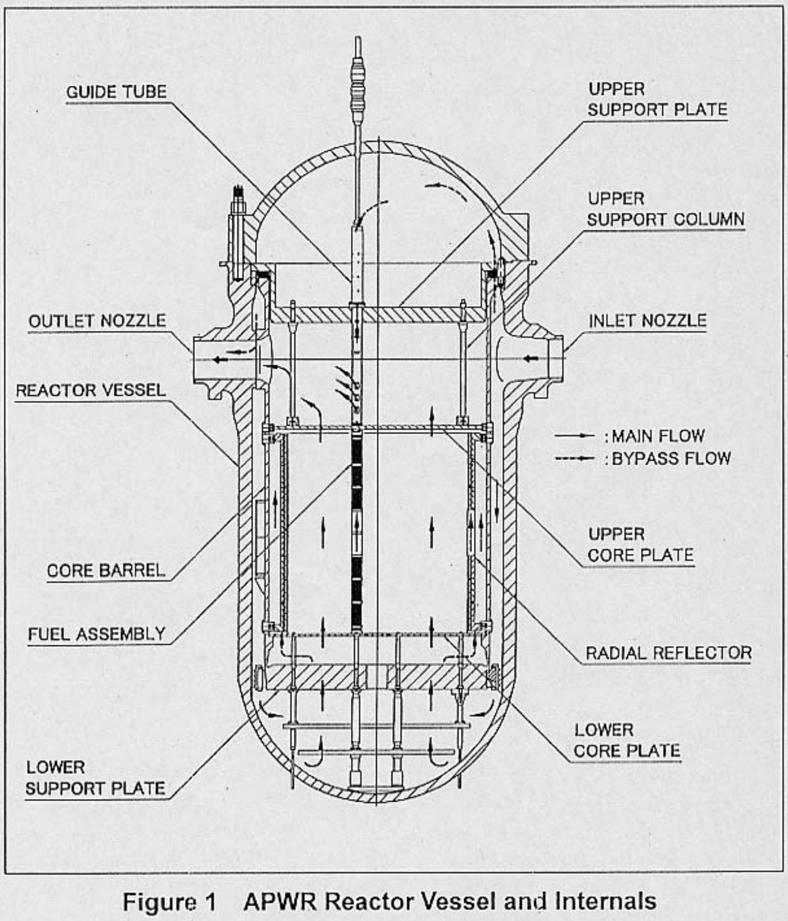


Figure 1 APWR Reactor Vessel and Internals

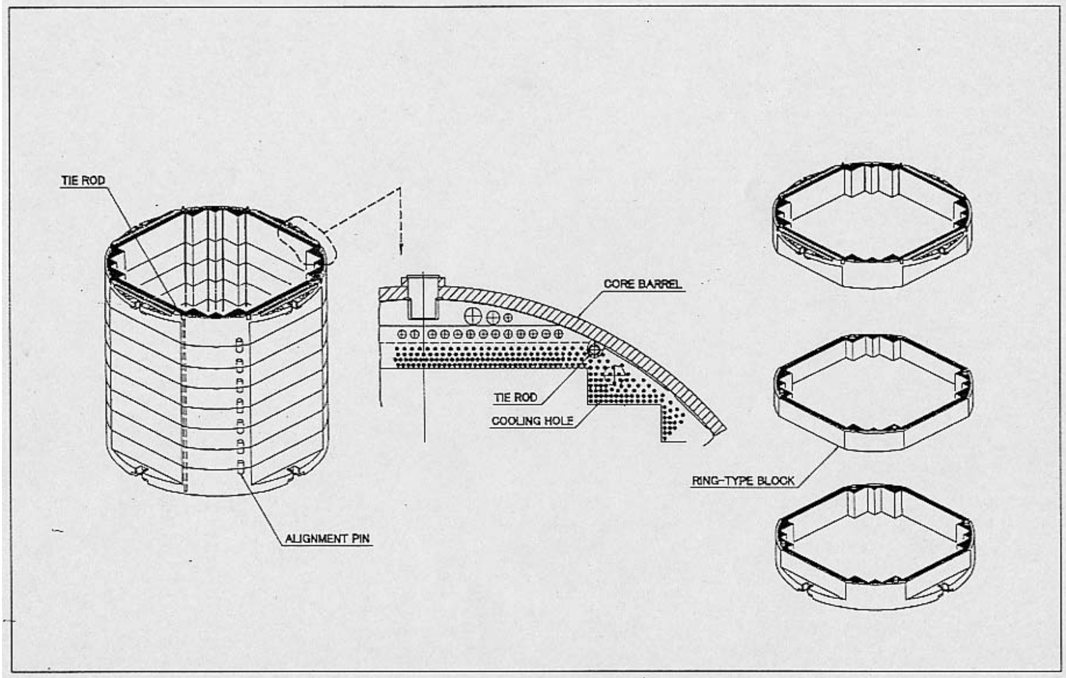


Figure 2 Configuration of APWR Radial Reflector

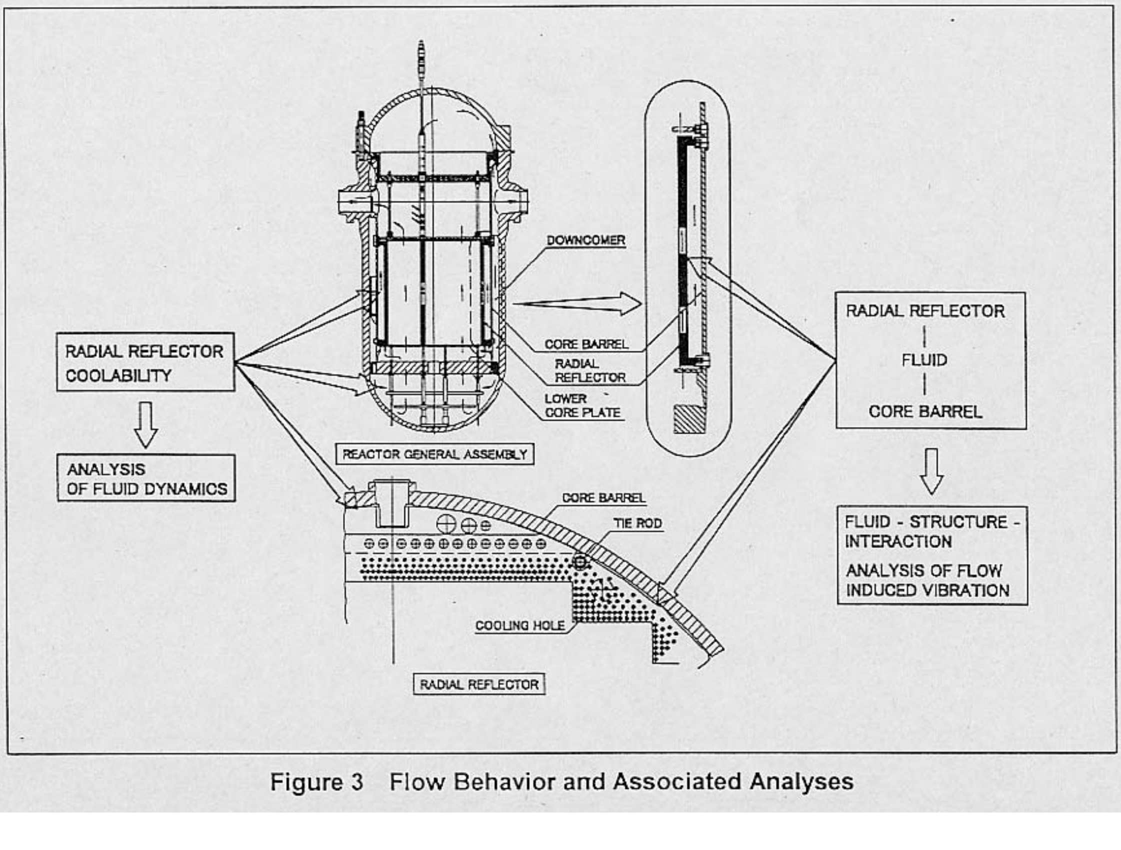


Figure 3 Flow Behavior and Associated Analyses

Flow induced vibration of APWR radial reflector

Relevance of the phenomenon as far as NRS is concerned
Flow-induced vibrations of the radial reflectors in APWRs could result in fretting, and possibly rupture, of the fuel pin cladding

What the issue is
If the core barrel is vibrated by the turbulent flow in the downcomer, it vibrates the radial reflector through the water between them (Fig.4). If the radial reflector vibrates, the grid of the outermost fuel bundles may make contact with it, and when the grid vibrates, the fuel clad may be worn out.

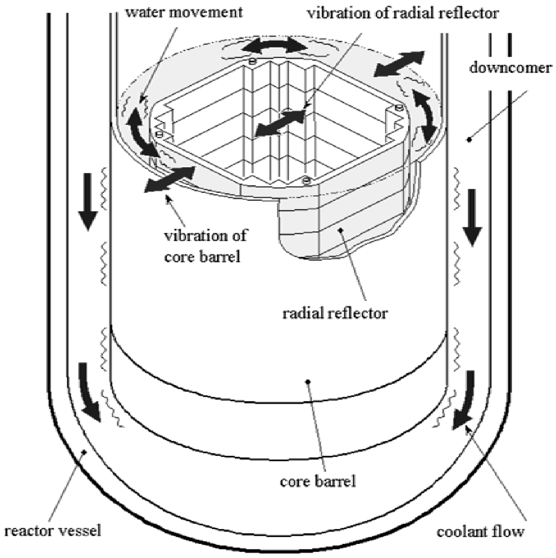


Figure 4. **Flow-induced vibration of radial reflector**

What the difficulty is and why CFD is needed to solve it
In order to evaluate the vibration of the radial reflector with sufficient accuracy, it is necessary to calculate the pressure fluctuations of the turbulent flow in the downcomer correctly, which is the driving force of the vibration. The following two methods are available for using CFD for evaluating the vibration between fluid and structure; the latter method is more practical.

(1) The vibration between fluid and a structure is calculated directly by the coupled use of a CFD code and a structural analysis code, using the moving boundary technique.

(2) The vibration between fluid and a structure is calculated by the structural analysis code, modelling the water between the core barrel and the radial reflector as simply an additional mass, and imposing the downcomer pressure fluctuations calculated by the CFD code as load conditions.

What has been attempted/achieved so far and what needs to be done
The vibration between fluid and structures has been calculated using the structural analysis code FELIOUS. The distribution of the downcomer fluid pressure fluctuations, which is used as the load conditions in the input data of the FELIOUS code, is obtained from a statistical analysis of the

experimental data of the 1/5-scale APWR test facility. Moreover, the 3-dimensional transient analysis of the turbulent flow in the downcomer has been carried out using a CFD code with LES (Large Eddy Simulation) turbulence model, and the calculated results have been compared with the above mentioned experimental data. The application of the LES model with high accuracy to the large calculation system of several orders of magnitude difference in scale is needed.

Ref. 1: F. Kasahara, S. Nakura, T. Morii, Y. Nakadai, *"Improvement of hydraulic flow analysis code for APWR reactor internals"*, CFD Meeting in Aix-en-Provence, May 15-16, 2002, NEA/CSNI/R(2002)16.

Natural circulation in LMFBRs

Relevance of the phenomenon as far as NRS is concerned
Current LMFBR designs often feature passive devices for decay-heat removal. It is necessary to demonstrate that the system operates correctly under postulated accident conditions.

What the issue is
Decay heat removal using natural circulation is one of the important functions for the safety of current LMFBRs. For example, DRACS (Direct Reactor Auxiliary Cooling System) has been selected for current designs of the Japanese Demonstration Fast Breeder Reactor. DRACS has *Dumped Heat Exchangers* (DHXs) in the upper plenum of the reactor vessel. Cold sodium provided by the DHX covers the reactor core outlet, and also produces thermal stratification in the upper plenum (Fig.1). In particular, the decay heat removal capability has to be assured for the total blackout accident in order to achieve high reliability.

What the difficulty is and why CFD is needed to solve it
The cold sodium in the upper plenum can penetrate into the gap region between the subassemblies due to negative buoyancy, and enhances the natural convection in these gap regions. Analyses of natural circulation tests in the Japanese experimental reactor JOYO revealed that heat transfer between subassemblies, i.e. inter-subassembly heat transfer, reduced subassembly outlet temperatures for the inner rows of the core. CFD is effective in evaluating the complex flow field caused by natural convection in the LMFBR reactor vessel.

What has been attempted/achieved so far and what needs to be done
The three-dimensional flow field and temperature distribution of sodium in the reactor vessel have been evaluated by JNC (Japan Nuclear Cycle Development Institute) using the CFD code AQUA.

The three-dimensional natural convection in the reactor vessel, coupled with the one-dimensional natural circulation in the loops, have been evaluated simultaneously by JAPC (Japan Atomic Power Company) using a CFD code combined with a system code.

Ref. 1: H. Kamide, K. Hayashi, T. Isozaki, M. Nishimura, "Investigation of Core Thermohydraulics in Fast Reactors - Interwrapper Flow during Natural Circulation", *Nuclear Technology,* 133, 77-91 (2001).

Ref. 2: H. Kamide, K. Nagasawa, N. Kimura, H. Miyakoshi, "Evaluation Method for Core Thermohydraulics during Natural Circulation in Fast Reactors (Numerical Predictions of Inter-Wrapper Flow)", JSME International Journal, Series B, Vol.45, No.3, 577-585, 2002.

Ref. 3: Watanabe et al., "Study on Natural Circulation Evaluation Method for a large FBR", Proc. NURETH-8 Conference, Kyoto September 30 - October 4, 1997.

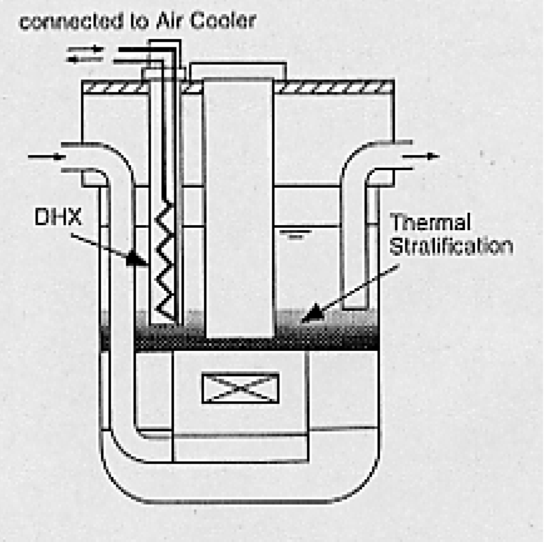


Fig. 1 Schematic of DRACS

Natural Circulation in PAHR (Post Accident Heat Removal)

Relevance of the phenomenon as far as NRS is concerned

Following a loss of core geometry as a consequence of a severe accident in an LMFBR, the availability of the decay heat removal systems have to be guaranteed to prevent possible melt-through of the reactor vessel.

What the issue is

After a core disruptive accident in an LMFBR, molten core material is quenched and fragmented in the sodium and settles to form a debris bed on structures in the reactor vessel. If the decay heat generated within the debris bed is not removed over a long period of time, the debris bed could melt again, and cause failure of the reactor vessel.

What the difficulty is and why CFD is needed to solve it

Decay heat in the debris bed is removed by natural convective flows passed through several leak paths which do not exist under normal operation conditions in current designs of Japanese Demonstration Fast Breeder Reactor (Fig.2). CFD methods are effective in evaluating the above-mentioned complicated natural circulation flow to high accuracy.

What has been attempted/achieved so far and what needs to be done

The 3-dimensional natural circulation flow in the above-mentioned situation has been evaluated using a state-of-the-art CFD code. (There is no open report).

Ref. 1: K. Chitose *et al*., *"Post Accident Heat Removal for a large LMFBR Core (in Japanese)"*, Fall Meeting of Atomic Energy Society of Japan, Nagoya, Japan, Oct., 1992.

Ref. 2: H. Arikawa, K. Tanimoto, K. Chitose *et al*., *"Test and Analysis of Decay Heat Removal Evaluation for Core Disruptive Accident for FBR (in Japanese)"*, 37th Heat Transfer Symposium of Japan, Kobe, Japan, May 2000.

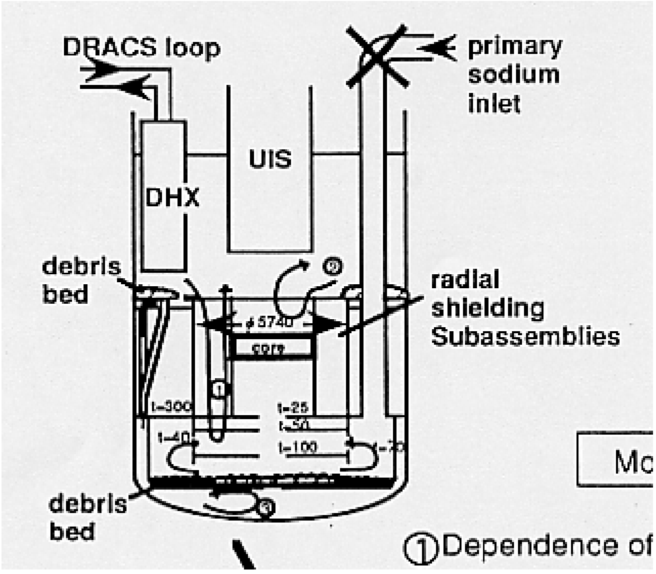


Figure 2: Schematic of the Demonstration Fast Reactor

Gas Flow in the Containment following a Sodium Leak

Relevance of the phenomenon as far as NRS is concerned
The sodium coolant used in LMFBRs is a hazardous material, and adequate precautions have to be made if a spill occurs.

What the issue is
Liquid sodium has preferable characteristics as a coolant in LMFBRs from both the neutronics and thermal-hydraulics viewpoints. On the other hand, liquid sodium will chemically react with oxygen or water if it leaks out of heat transport system. For the safety of the LMFBR plants, it is important to evaluate the consequence of possible sodium combustion.

What the difficulty is and why CFD is needed to solve it
Leaked sodium may break up into small droplets of various diameters. In an air atmosphere, the droplets burn as they fall. This is designated as spray combustion. The unburned sodium collects on the floor of the reactor building, and pool combustion may ensue (Fig.3).

In order to evaluate the spray combustion rate with sufficient accuracy, it is necessary to evaluate the amount of oxygen which flows around the sodium droplets. The amount of oxygen depends on the gas flow in the room caused by the motion of sodium droplets, and the temperature/concentration stratification.

On the other hand, in order to estimate the pool combustion rate with sufficient accuracy, it is necessary to evaluate the amount of oxygen which flows to the sodium pool surface. This depends on the natural convection flow generated on the hot pool surface. A CFD code is effective in evaluating this gas flow.

What has been attempted/achieved so far and what needs to be done
The CFD code AQUA-SF has been developed by JNC (Japan Nuclear Cycle Development Institute) to evaluate spatial distributions of gas temperature and chemical species. The code includes the spray combustion model and a flame-sheet pool combustion model.

Ref. 1: A. Yamaguchi, T. Takata, Y. Okano, *"Numerical Methodology to Evaluate Fast Reactor Sodium Combustion"*, Nuclear Technology, 136, 315-330, (2001).

Ref. 2: T. Takata, A. Yamaguchi, I. Maekawa, *"Numerical Investigation of Multi-dimensional characteristics in sodium combustion"*, Nuclear Engineering and Design, 220, 37-50 (2003).

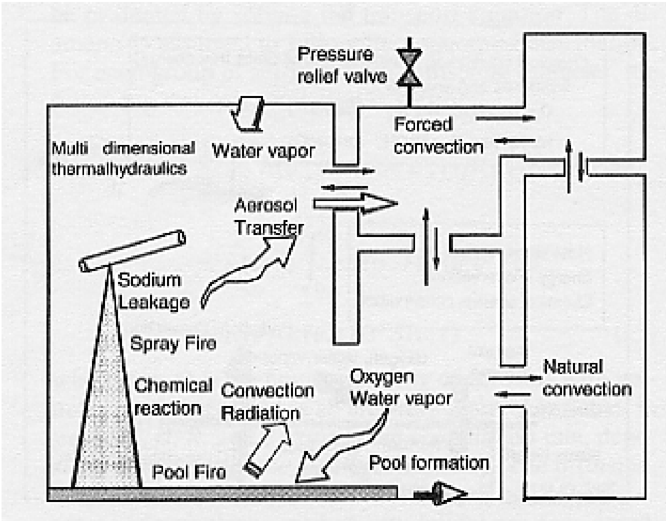


Figure 3**:** **Computational Models for the SPHINCS Program**

AP600

Relevance of the phenomenon as far as NRS is concerned
The AP600 is a 2 loop PWR, designed by Westinghouse, with passive safeguard systems. The passive safety systems, such as core makeup tanks and the passive residual heat removal heat exchanger, depend on gravity, and the availability of these components should be confirmed under accident conditions.

What the issue is
The AP600 has several passive system components, and thermal-hydraulic phenomena relating to these components will occur during accidents or transients: thermal stratification in the core makeup tank (CMT), downcomer and cold legs, condensation and convection in the in-containment refuelling water storage tank (IRWST), and so on.

In the IRWST, three-dimensional thermal convection due to the heat transfer from the passive residual heat removal (PRHR) heat exchanger, and the condensation of steam from the automatic depressurisation system (ADS), are both important for cooling of the primary system.

Thermal stratification in cold legs is one of the significant phenomena under some small-break LOCA conditions after the termination of the natural circulation through the steam generators. In the loop where the PRHR system is connected, the fluid in the cold leg is a mixture of the draining flow from the steam generator U-tubes and the discharge from the PRHR heat exchanger in low-temperature IRWST, and becomes significantly colder than the downcomer liquid. The relatively warmer downcomer liquid intrudes along the top of the cold leg. In contrast, in the loop with the CMT, the cold-leg liquid is kept at a higher temperature than the downcomer liquid temperature, since the CMT water is injected into the downcomer through the direct vessel injection (DVI) line, and the downcomer liquid intrudes along the bottom of the cold leg. In both cases, a counter-current flow is established as well as the thermal stratification. In case of cold-leg break LOCAs, the thermal stratification in the cold legs has an effect upon the discharge flow rate from the break point, and thus the system response.

What the difficulty is and why CFD is needed to solve it

Three-dimensional convection in a tank, and counter-current thermal stratification in legs, are difficult to model using system analysis codes based on one-dimensional components. The difference of discharge from a break point due to the difference of orientation is not generally accounted for. The system behaviour, however, is associated with these local phenomena, and a CFD approach is necessary for safety evaluation of new types of components and reactors.

What has been attempted/achieved so far and what needs to be done

Three-dimensional calculations for single-phase flows are possible using commercial CFD codes. The cold-leg flow, however, becomes a two-phase mixture under some conditions, and is much influenced by the system response. The flow in the IRWST is also related strongly to the system response. Detailed three-dimensional calculations of single- and two-phase flows are necessary at the same time with, or in the framework of, the system analyses.

Ref. 1: http://www.iaea.or.at/programmes/ne/nenp/nptds/newweb2001/simulators/cti_pwr/pwr_ap600_overview.pdf

SBWR, ESBWR and SWR-1000

Relevance of the phenomenon as far as NRS is concerned

Evolutionary-design reactor systems often feature passive decay-heat removal systems, including passive decay heat removal from the containment in the event of a LOCA. The coupling of the primary circuit and containment response is a new concept, and needs to be thoroughly understood in order to ensure safe operation of the reactor under such conditions.

What the issue is

The phenomena to be investigated involve mixing and transport of the containment gases — steam and non-condensables (nitrogen and, in the case of severe accidents involving core degradation, possibly also hydrogen) — and condensation of the steam on cold surfaces and/or water pools.

What the difficulty is and why CFD is needed

Generally, in all the above cases, decay heat removal involves complex mixing and transport of two-component/two-phase flows in complex geometries. The numerical simulation of such behaviour requires the use of sophisticated modelling tools (i.e. CFD) because of the geometric complexities and the inherent 3-D behaviour, together with the development of reliable and appropriate physical models.

The principles, which reflect the need for advanced tools, may be illustrated with reference to the schematic of the ESBWR shown in Fig. 4a. The Drywell is directly connected to Passive Containment Cooler (PCC) units, which sit on the containment roof. The steam condensed in these units is fed back to the Reactor Pressure Vessel (RPV), while any uncondensed steam, together with the nitrogen which originally filled the Drywell atmosphere, is vented to the Suppression Pool. Clearly, partial condensation of steam and stratified conditions in the pool are both unfavourable, leading to excess pressure in the chamber. It is therefore important to understand the condensation and mixing phenomena which occur in the pool. To accurately represent the dynamics of the bubble expansion and break-up, CFD, in combination with an interface tracking procedure (e.g. VOF or LS) is required.

Following break-up of the primary discharge bubble into smaller bubbles, it is no longer convenient to explicitly describe the liquid/gas interface, because of its disjointedness and complexity. Consequently, an Euler/Euler, two-fluid approach has been followed, with the water acting as the continuous medium and the bubbles representing the dispersed phase. A full description of the bubble dynamics, and the stirring of the water in the pool to break up stratified layers, will encompass CFD with two-phase flow and turbulence models.

In the SWR-1000 (Fig. 4b), containment condensers are employed. One condenser under consideration is a cross-flow, finned-tube heat exchanger with steam condensation outside the tubes and water evaporation within. The tubes are slightly inclined and staggered (Fig. 5). The performance of such finned tube containment condensers can be investigated at small and medium scale, but the scaling factors remain uncertain for a full-sized unit. CFD offers an opportunity to analyse the full-scale situation cheaply and efficiently, using data from smaller tests to validate the models.

What has been attempted and achieved/what needs to be done (recommendations)
Aspects of the issues alluded to above have been tackled using CFD methods in the context of the EU shared-cost actions TEMPEST, IPSS, INCON and ECORA. In addition, CFD has been used to model the mock-up experiments carried out in the PANDA facility. Considerable modelling effort has been expended on condensation in the presence of non-condensables, interface tracking of gas-discharge bubbles and bubble plumes in suppression pools. Requiring more attention is the extension of the two-phase CFD models for condensation and turbulence.

Ref. 1: S. Rao, A. Gonzalez, 1998, *"ESBWR: Using Passive Features for Improved Performance and Economics"*, Proc. Nucl. Conf., Nice, France, 26-28 Oct. 1998.

Ref. 2: G. Yadigaroglu, 1999, *"Passive Core and Containment Cooling Systems: Characteristics and State-of-the-Art"*, Keynote Lecture, NURETH-9, 3-8 Oct., 1999.

Ref. 3: N. S. Aksan, and D. Lubbesmeyer, *"General Description of International Standard Problem 42 (ISP-42) on PANDA Tests"*, Proc. Int. Conf. ICONE9, Nice, France, April 8-12, ASME/JSME/SFEN, 2001.

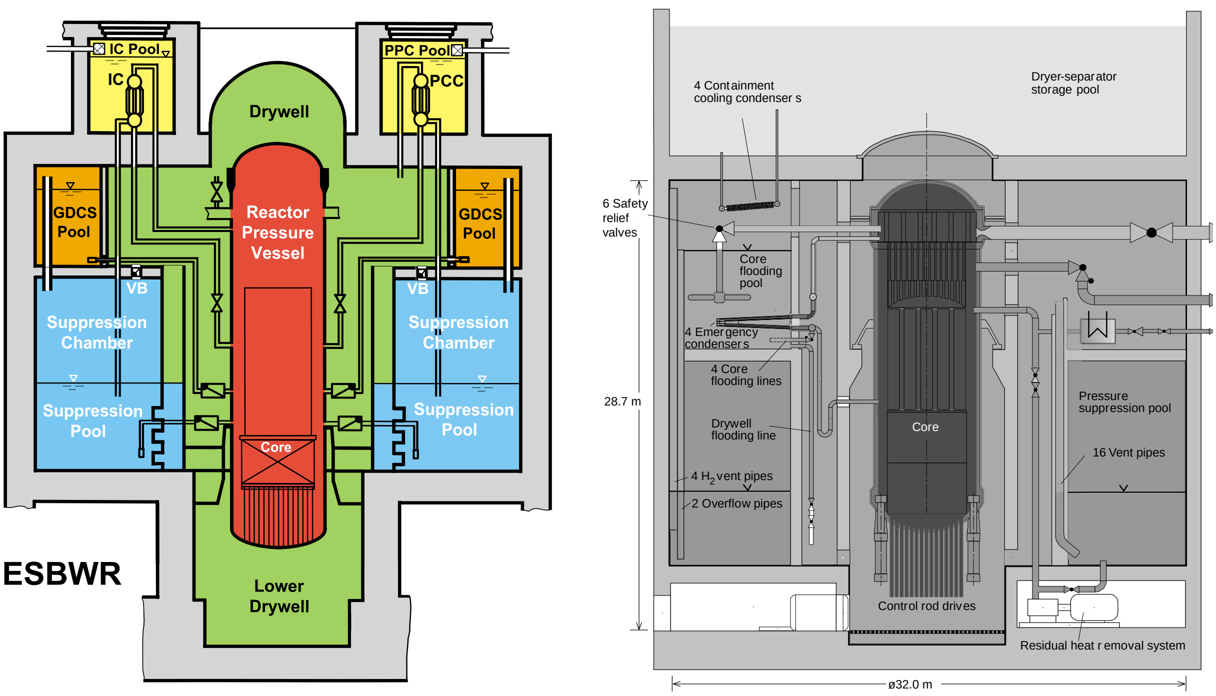


Figure 4: **Two Evolutionary Reactor Designs: (a) ESBWR, (b) SWR-1000**

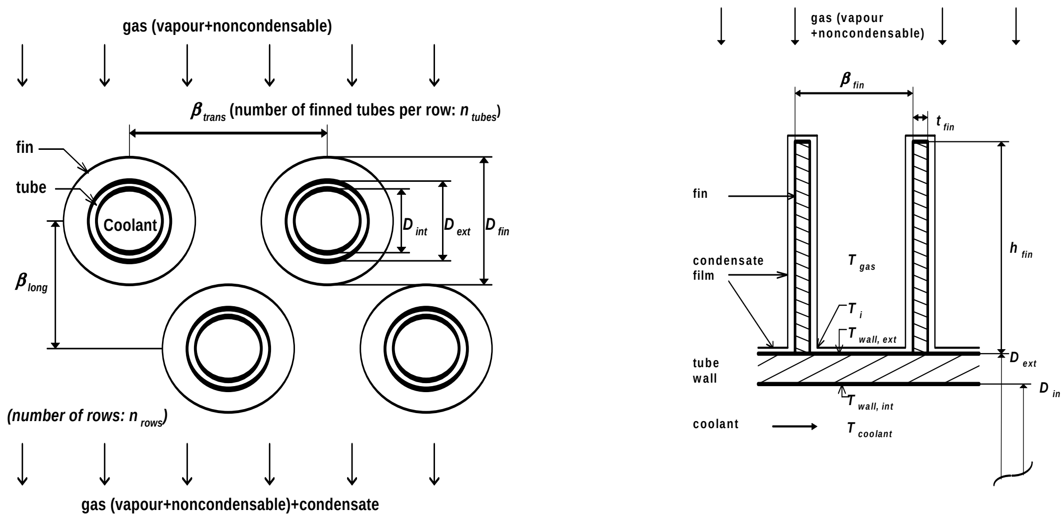


Figure 5: **Bundle and Finned Tube geometries**

High Temperature Gas-Cooled Reactor

Relevance of the phenomenon as far as NRS is concerned
The relevant part of the HTGR as far as NRS is concerned may be the containing vessel as well as the whole circuit, including the lower and upper plena, the power conversion system (for direct Brayton Cycle) and the core. One principal concern is that, for most of the accident scenarios for these reactors, safety relies on a passive system of residual power release. For other cases, such as “abrupt power rise” and even LOCA, NRS relies on the beneficial effect of thermal core inertia (graphite), the eventual power release being ensured by radiation transfer from the core to the vessel walls. This perspective relies on the behaviour of the core at high temperatures (triso-particle).

What the issue is
The issues depend on the precise part of the reactor under consideration.

1. *Primary Loop Ducts*. The NRS scenario may concern breaks in ducts that may lead to air ingress and possible air/graphite interaction.

2. *Containing Vessel*. The basic issue here is to precisely determine the global heat transfer between the core and the vessel walls, resulting from both natural convection and radiation. The two main issues are to check the capability of the system to remove all power while preserving the vessel integrity, and to identify the hot spots.

3. *Lower Plenum*. One of the basic issues is the reliance placed on the calculation of the flow behaviour in the lower plenum: for example, in column matrices (Ref. 1). The main physics relies on the capability of the system to mix flows of different temperatures to avoid temperature fluctuations on support structures, as well as at the turbine inlet.

4. *Upper Plenum*. First issue is related to Item 1 (heat release through radiation process), and the second issue concerns temperature fluctuations on internal structures.

5. *Turbine.* First issue is connected with Item 2 (temperature heterogeneity at the inlet for nominal and accident scenarios). Second issue concerns the temperature of the blades and disks. Indeed, these structures may not be cooled in some designs. For all the transients where these structures are not cooled, the question of thermal constraints arises. Other issues concern the dynamical behaviour: pressure variation, rotating speed variation, etc.

6. *Compressor.* Particular regimes such as stall or surge in the case of depressurisation may be of concern.

7. *Heat exchanger*. Firstly, the water exchangers are the only cold source of the primary loop. They should be checked for many transient situations: e.g. loss of load, pre-cooler failure, etc. NRS scenarios may also concern secondary loop water ingress. Secondly, the heat recuperator is submitted to temperature and pressure fluctuations at inlet.

8. *Core*. The core is subject to the usual problems, such as power rise, LOCA, etc.

What the difficulty is and why CFD is needed

Geometries are complex, and it is difficult to make simplifications to ease modelling. Transients (which may be short or very long) involve multi-physics phenomena: CFD has to be employed in combination with conjugate heat transfer, radiation and neutronics coupling, for example, and the flow regimes are varied and complex (from incompressible to compressible, from laminar to turbulent – and sometimes with relaminarisation – and from forced to mixed and natural convection).

CFD is required, or is at least preferable, in the following circumstances.

- Where real three dimensional flows occur, which is typically the case for:
  - the core in accident situations (tube plugging or power rise);
  - the lower plenum, since asymmetrical flow develops due to the position of the outlet; and
  - the heat exchanger, though here the case for CFD is questionable, since such a component can be taken into account only at the system level; however, a precise description of the phenomena may require CFD.
- Where complex flows develop in situations in which details of local quantities or local phenomena are needed. This is the case for:
  - the turbine, where local information about hot spots is required;
  - the compressor, where stall prediction is an issue; and
  - generally, where local values are needed for the determination of hot spots.
- Even if the global behaviour in the upper plenum may be described as a component through a 0-D system approach, CFD may produce a more accurate description of the mixing processes occurring as a result turbulence action.
- The precise description of local effects may be of relevance in the case of air ingress prediction, thermal fatigue (the GCR counterpart of the PWR tee-junction or thermal shock problem).

What has been attempted and achieved/what needs to be done (recommendations)
Pioneering simulations concerning flows around lower plenum columns, and flows in some regions of the core, have been conducted at CEA (Ref. 2).

Ref. 1: Tauveron, N. *"Thermal fluctuations in the lower plenum of a high temperature reactor"*, Nuclear Engineering and Design, 222, 125-137 (2003).

Ref. 2: Tauveron, N., Elmo, M., Cioni, O., Chataing, T. "*Thermohydraulic simulations on high temperature reactor"*, Proceedings of High Temperature Reactors Technology (HTR'2002), April 22-24, 2002, Petten, The Netherlands.

Ref. 3: E. Studer *et a*l., *"Gas Cooled Reactor Thermal-Hydraulics using CAST3M and CRONOS2 codes"*, Proc. 10th Int. Topical Meeting on Nuclear Thermal-Hydraulics, NURETH-10, Seoul, Korea, 5-11 October 2003.

4. IDENTIFICATION OF EXISTING ASSESSMENT BASE

Background

Major sources of information identified by the Group are elaborated below under appropriate section headings. In addition, in summary form, references to documents available from the NEA/CSNI and elsewhere are collected at the end of the section.

Some of the web sites referenced below allow free access to data for code validation, they sometimes propose CFD reference calculations, and they ask people to participate to the enhancement of the database by submitting their own cases. In this way, the CFD community has ready access to an ever increasing body of information to act as an assessment base for their activities. At present, the activities are orientated primarily towards the aerospace and aerodynamics communities, but at least demonstrate the seriousness of the commitment to "quality and trust" in CFD, and the concept could be expanded to serve the nuclear community also.

Ref. 1: *"Verification and Validation of CFD Simulations"*, 1999, Stern, Wilson, Coleman, Paterson (Iowa Institute of Hydraulic Research and Propulsion Research Center), report of the IIHR, (www.iihr.uiowa.edu/gothenburg2000/PDF/iihr_407.pdf).

Ref. 2: *"Verification and Validation in Computational Fluid Dynamics"*, 2002, Oberkampf, Trucano, Sandia National Laboratories report.

Ref. 3: *"Tutorial on CFD V&V of the NPARC Alliance"* (http://www.grc.nasa.gov/WWW/wind/valid/validation.html).

4.1 ERCOFTAC

The European Research Community on Flow, Turbulence And Combustion (ERCOFTAC) is an association of research, educational and industrial groups with main objectives to promote joint efforts, centres and industrial application of research, and the creation of Special Interest Groups (SIGs). The home page is www.ercoftac.org.

A large number of SIGs have been formed, and one is the ERCOFTAC Database Interest Group (DBig), with the objective to coordinate, maintain and promote the creation of suitable databases derived from experimental, DNS, LES, CFD, PIV and flow visualisation specialists.

This data base, started in 1995, and administrated by UMIST Mechanical Engineering CFD group, contains experimental as well as existing numerical data (collected through Workshops) relative to both academic and more applied applications.

The database is actively maintained by UMIST staff, and is currently undergoing a restructuring and expansion to include, amongst other things, more details of the test cases, computational results, and results and conclusions drawn from the ERCOFTAC Workshops on Refined Turbulence Modelling. Each case contains at least a brief description, some data to download, and references to published work. Some cases contain significantly more information than this.

In addition to the flow case descriptions and data, there are also a number of discussion forums available. These allow users to make their own contributions by posting their own findings, questions or answers on particular cases. The database is open worldwide. However, to enable the organisers to keep track of how the database is being used, it is necessary to register.

The website address to the ERCOFTAC Classic Database Collection is http://cfd.me.umist.ac.uk/ercoftac/)

4.2 QNET-CFD

QNET-CFD is “A Thematic Network for Quality and Trust in the Industrial Application of Computational Fluid Dynamics” within the GROWTH programme of the EU; Prof. Charles Hirsch (Vrije Universiteit Brussel) is the project coordinator. According to the basic network document (Annex 1), “The Network sets out to assemble, structure and collate existing knowledge, encapsulating the performance of models underlying the current generation of CFD codes, and to make this information available in the form of a knowledge base.”

The 3rd QNET-CFD Workshop took place in Prague (Czech Republic), May 29-30, 2003, and a complete agenda of the meeting is available online at http://www.qnet-cfd.net/events.html.

Presentations included:

- AIAA Committee on Standards for Computational Fluid Dynamics - Verification Project Status and Plans, Chris Rahaim, St. Louis University, USA
- The A aerofoil: incipient separation at maximum lift, Peter Voke, University of Surrey, UK
- Turbulence modelling of an axisymmetric jet impinging on a heated flat plate, Remi Manceau, Université de Poitiers, France
- 2D backward facing step, Javier Principe, CIMNE, Spain.
- Laminar-turbulent boundary layer transition, Witold Elsner, Technical Univ., Czestochowa, Poland.
- Confined buoyant plumes, Darren Woolf, Arup, UK.

- Numerical solution of some problems of external and internal aerodynamics with applications, Karel Kozel. Czech Academy of Sciences.

- Accurate prediction of diffuser flows: a status report, Florian Menter, AEA Technology, Germany.

- Transonic flows in some turbine cascades, J. Fort K. Kozel, J. Prihoda, P. Safarik, Czech Academy of Sciences

Several very interesting presentations from the 2nd QNET-CFD Workshop are now also available online as PDF files from the QNET-CFD web site.

The fourth and final Workshop was held in May 13-14, 2004, and proceedings will be available within the public section of the web page. The databases for the different Thematic Areas will be made available through ERCOFTAC. Dr. Chris Lea, who has been the coordinator of TA-3 “Thematic Area on Chemical and Process, Thermal Hydraulics & Nuclear Safety”, will also continue to have a coordinating role in this area. It is expected that new test cases will be added to the databases. At Workshop 4, each TA coordinator also gave BPA presentations.

During the course of QNET-CFD, each Thematic Area coordinator produced state-of-the-art reviews related to the application and validation of CFD in the respective areas. At present, these reports are available only to members. In the last TA-3 report, the importance of validation for thermal hydraulics and the nuclear industry is stressed, and it is pointed out that, for example, flows such as free, mixed and forced convection are typical cases for which simple turbulence models and wall functions perform badly.

Application challenges submitted in TA-3 are listed below:

- Buoyancy-opposed wall jet

- Induced flow in a T-junction

- Cyclone separator

- Flow through textile fabric

- Buoyant gas/air mixing in a vessel

- Mixed convection in a vessel

- Gas release from high-pressure pipelines

- Spray evaporation in turbulent flow

- Natural convection in a horizontal pipe

- Combining/dividing flow in a junction

- Downward flow in heated annulus

A brief overview of key physical processes requiring modelling, and modelling approaches, is also given in one chapter.

The "knowledge base" of QNET-CFD contains "Application Challenges" for each Thematic Area, and also "Underlying Flow Regimes" (UFRs). Each application is structured, with chapters for description, test date, CFD simulations, evaluation and practise advice (BPA). How it best relates to underlying flow regimes is covered in a separate chapter. UFRs for combustion and multiphase flows are still missing. Recommendation for future work is also given.

It should also be mentioned that it is not only TA-3 that is of interest for WG2, also the other thematic areas and the underlying flow regimes have important information and advice, and all are well-structured.

4.3 MARNET

These are Best Practices Guidelines for Marine Applications of CFD, and were prepared by WS Atkins Consultants. The general ERCOFTAC document is taken as a starting point, and specific advice on the application of CFD methods within the marine industry are provided.

Full details are contained in the WG1 document.

4.4 FLOWNET

The FLOWNET initiative is intended to provide the scientific and industrial communities with a code validation tool for flow modelling and computational/experimental methods. By means of network databases, multi-disciplinary knowledge is cross-fertilised and archived. Providing a share of technical complements to scientists and engineers, the network enhances quality and trust in pre-industrial processes. The ultimate goal of the network is to bring together academic and industrial node partners in a dynamically open forum to evaluate continuously the quality and performance of CFD software for improving complex design in industry from the viewpoint of accuracy and efficiency. The FLOWNET project provides data once specific authorisation has been provided; the main orientation is the aerodynamics community.

Ref. 1: http://dataserv.inria.fr/sinus/flownet/links/index.php3.

4.5 NPARC

The NPARC Alliance for CFD Verification & Validation provides a tutorial, as well as available measurements and data for CFD cases (both analytical and, particularly, orientated towards the aerodynamics community. The data set archive of NASA provides data for CFD applications.

Ref. 1: http://www.nas.nasa.gov/Software/DataSets.

4.6 AIAA

The American Institute of Aeronautics and Astronautics, or AIAA, is a 65-year-old "professional society for aerospace professionals in the United States". Its purpose it to "advance the arts, sciences, and technology of aeronautics and astronautics, and to promote the professionalism of those engaged in these pursuits". For example, there is a link up with the QNET-CFD activity (Ref. 1). The society participates to the definition of standards for CFD in its "Verification and Validation Guide".

Web sites related to AIAA activities (base web address http://www.aiaa.org) propose lists of references (papers, books, author coordinates) related to CFD verification and validation (see http://www.aiaa.org/publications/database.html) and various links with other web sites gathering information of aeronautical interest. Some of these links may provide valuable information for CFD validation (e.g. http://www.icase.edu/docs/library/itrs.html), though this would have to be sifted for information of interest to the NRS community.

Full details are contained in the WG1 document.

Ref. 1: http://www.qnet-cfd.net/workshop/1st/pdf/02_in-1_aiaa.pdf.

4.7 Vattenfall Database

The Plane Wall Jet (UFR3-10)
Detailed three-component turbulence measurements in a wall jet down to $y^+<2$ are reported. The experimental technique was a combination of light collection in 90° side-scatter, and the use of optics with probe volumes of small diameters. A complete k-profile was obtained, and turbulence statistics up to fourth order are presented for all three velocity components. Comparing the wall jet to the flat plate boundary layer, one finds that the turbulence structure in the near-wall region is qualitatively very similar, but that the actual values of the quantities (in conventional inner scaling) are higher for the wall jet.

Draft Tube (TA6-07) for a Kaplan Turbine
Data have been made available from measurements taken using LDV in a model turbine (scale 1:11) at Vattenfall Utveckling, Älvkarleby, Sweden for an ERCOFTAC/IAHR sponsored Workshop: Turbine 99 - Workshop on Draft Tube Flow, held at Porjus, Sweden on 20-23 June, 1999. The basic challenge for calculations submitted to the Workshop was to predict technically relevant quantities from measured data at the inlet and outlet of the draft tube. This involved head loss coefficients, pressure distributions and the positions of separated flow regions. A substantial amount of additional experimental data was made available to the participants at the meeting, involving velocity fields at several internal points, boundary layer profiles at selected points, and visual observations (with laser-induced fluorescence) of swirl and recirculation zones. Proceedings of the Workshop are available on the web at http://www.sirius.luth.se/strl/Turbine-99/index.htm, and the benchmark is also referenced in QNET-CFD.

Ref. 1: Eriksson J; Karlsson R; Persson J *"An Experimental Study of a Two-Dimensional Plane Turbulent Wall Jet"*, Exp. Fluids, **25**, 50-60 (1998).

Ref. 2: Andersson, U., Karlsson, R., *"Quality aspects of the Turbine-99 experiments"*, in Proceedings of Turbine-99 – Workshop on draft tube flow in Porjus, Sweden, 20-23 June 1999.

Ref. 3: The QNET-CFD Network Newsletter, A Thematic Network For Quality and Trust, Volume 2, No. 3 – December 2003.

4.8 Jahrestagung Kerntechnik

Below is a list of recent publications from the journal, which demonstrate the increasing use of CFD in the nuclear technology field.

Braun, T., Koch, M. K, Unger, H.: *"Vorausrechnung eines Thermohydraulik-Versuchs in der ThAI-Anlage mit dem Programmsystem COCOSYS V2.0v1"*, 2003.

Batta, A., Grötzbach, G., Cheng, X.: *"CFD analysis of the flow behaviour in a spallation target"*, 2003.

Ganzmann, T. I., Meseth, J., Bielor, E. , Freudenstein, K. F., Roth, F. , H. Schmidt, H.: "*Tests and calculations to investigate the in-core boron distribution of the Fast Acting Boron Injection System of the SWR 1000"*, 2003.

Schulenberg, T., Meyer, L., Alsmeyer, H.: *"Status on research about ex-vessel corium release and retention"*, 2003.

Meyer, L., Albrecht, G., Kirstahler, M., Schwall, M., Wörner, G., Wachter, E.: *"Curium dispersion and direct containment heating experiments at low pressure"*, 2003.

Fischer, U., Gordeev, S., Heinzel, V., Schleisiek, K., Simakov, S., Slobodtchouk, V., Stratmanns, E.: *"Optimized Design of the High-Flux-Test-Module for the International-Fusion-Material Irradiation-Facility"*, 2003.

Esser, F., Glückler, H., Hansen, G., Krauthausen, W., Lennartz, M., Wolters, J., Wolters, J. P.: *"Auslegung eines Behälters zur Reduzierung der N-16 Aktivität im Kreislauf der Bestrahlungseinrichtung BE46 im FRJ-2 der Forschungszentrum Jülich GmbH"*, 2003.

Stratmann, W., Wortmann, B.: "*Strahlenschutz und Lüftungstechnische Berechnung von Abschirmschrauben"*, 2003.

Laurien, E.: "*The numerical simulation if three-dimensional two-phase flows as a tool for light-water reactor design and safety analysis"*, 2002.

Rehm, W.: "*Fluid dynamic studies of combusting flows for hydrogen safety technology"*, 2002.

Giese, T., Laurien, E.: *"A gravity driven pipe flow with phase change phenomena"*, 2001.

Krepper, E., Hicken, E.-F., Jaegers, H.: *"Investigations of natural convection in large pools during the heating up of the secondary side of an emergency condenser"*, 2001.

Becker, S., Laurien, E.: *"Numerical simulation of the convective heat transport in pebble beds at high temperatures"*, 2001.

Rehm, W.: *"Applied Computational Fluid Dynamics (ACFD) using high-performance supercomputing clusters (HSPC)"*, 2001.

Giese , T., Laurien, E.: *"A three dimensional numerical model for analysis of pipe flows with cavitation*", 2000.

Bieder, U., Calvin, Chr., Etmonot, Ph.: *"Towards large eddy simulations in nuclear technology"*, 2000.

Kliem, M.: *"3D flow simulations for a reactor core modelled as porous body using CFX-4.2"*, 2000.

Koebke, K., Ren, M.: *"CFD-Anwendungen in der Brennelementtechnik"*, 2000.

Carteciano, L.N., Wörner, M., Grötzbach, G.: *"Erweiterte Turbulenzmodelle für technische Anwendung von Flutan auf Naturkonvektion"*, 1999.

Krepper, E., Weiss, F.-P., Willschütz, H. G.: *"Calculations at a mixed convection flow benchmark using different CFD codes"*, 1999.

Höhne, T.: *"Numerical simulation of the coolant mixing in pressurized water reactors"*, 1999.

G. Janssens-Maenhout, G., Knebel, J., Müller, U.: *"Subcooled nucleate boiling in industrial cooling loops"*, 1998.

Reinders, R.: *"dreidimensionale transiente Berechnung der Borkonzentration im RDB nach einem DE-Heizrohrleck"*, 1998.

Aszodi, A.: *"Simulation der einphasigen Naturkonvektion auf der Sekundärseite der Noko Anlage mit dem CFD-Code CFX 4"*, 1997.

Freudenstein, K., Reinders, R.: *"3D Computational Fluid Dynamics analysis of cold plumes in a BWR reactor vessel"*, 1997.

Aszodi, A.: *"Simulation der transienten Naturkonvektion in einem seitlich beheizten Behälter"*, 1996.

Rieger, T., Bürger, M., Schatz, A.: *"Effects of natural convection in the RPV and the hot legs on the in-vessel coolability during severe PWR accidents"*, 1996.

4.9 Existing CFD Databases: NEA/CSNI and Other Sources

	Source	**Reference**
1	State-of-the Art Report (SOAR) on Containment Thermal-Hydraulics and Hydrogen Distribution	NEA/CSNI/R(1999)16
2	SOAR on Flame Acceleration and Deflagration-to-Detonation Transition in Nuclear Safety	NEA/CSNI/R(2000)7
3	Proceedings of the May 1996 (Winnipeg) Workshop on the Implementation of Hydrogen Mitigation Techniques	NEA/CSNI/R(1996)8
4	Summary and Conclusions of the May 1996 (Winnipeg) Workshop on the Implementation of Hydrogen Mitigation Techniques	NEA/CSNI/R(1996)8
5	Proceedings of the 1996 (Annapolis) Workshop on Transient Thermal-Hydraulic and Neutronic Code Requirements	NEA/CSNI/R(1997)4
6	Proceedings of the April 2000 (Barcelona) Workshop on Advanced Thermal-Hydraulic and Neutronic Codes - Current and Future Applications (Volumes 1 and 2)	NEA/CSNI/R(2001)2
7	Summary and Conclusions of the April 2000 (Barcelona) Workshop on Advanced Thermal-Hydraulic and Neutronic Codes - Current and Future Applications	NEA/CSNI/R(2001)9
8	Proceedings of the May 2002 (Aix-en-Provence) Exploratory Meeting of Experts to Define an Action Plan on the Application of CFD to NRS Problems	NEA/CSNI/R(2002)16

	Source	Reference
9	Proceedings of the November 2002 (Pisa) IAEA/NEA Technical Meeting on the Use of Computational Fluid Dynamics Codes for Safety Analysis of Reactor Systems, Including Containment	NEA/CSNI/R(2003)
10	Severe Accident Research and Management in Nordic Countries -- A Status Report, May 2000	NKS-71 (2002)
11	NKS Recriticality Calculation with GENFLO Code for the BWR Core After Steal Explosion in the Lower Head, December 2002	NKS-83 ISBN 87-7893-140-1
12	The Marviken Full-Scale Experiments	CSNI Report No. 103
13	Analysis of Primary Loop Flows (ECORA WP2 Report)	http://domino.grs.de/ ecora/ecora.nsf

5. IDENTIFICATION OF GAPS IN TECHNOLOGY BASE

5.1 Isolating the CFD Problem

Reactor systems and containments are generally modelled as networks of 0-D and 1-D elements, with the systems represented by a series of control volumes connected by flow junctions; the system codes RELAP5, TRACE, CATHARE and ATHLET, for example, are constructed in this way. The flow conservation equations are applied to the volumes and junctions, and heat transfer and appropriate flow resistance correlations are imposed, depending on the flow regime. It is evident, however, that in some components the flow is far from being 1-D: for example, the flows in the upper and lower plena and downcomer of the RPV, and to some extent the core region, are all 3-D, particularly if driven by non-symmetric loop operation. Natural circulation and mixing in containment volumes are also 3-D phenomena.

It is inconceivable that CFD approaches will be able in the near future to completely replace the now well-established system code approach to analysing reactor transients. The number of meshes which would need to be employed would be well beyond the capabilities of present computers, closure relations for 3-D multi-phase situations are essentially non-existent, and criteria for defining flow regimes at the fine-mesh, CFD level is grossly underdeveloped, and no readily available CFD code has a neutronics modelling capability.

More useful would be to perform local CFD computations only where a fine-mesh resolution is required. The problems with this are that most of the interesting system behaviour is transient, and the local situation is strongly influenced by the system parameters.

More feasible is the possibility of interfacing a CFD module to an existing system code in order to perform a localised 3-D computation within the framework of an overall 1-D description of the circuit. This arrangement is attractive in that it retains the accumulated experience and reliability of the traditional system code approach, but extends its capabilities in modelling 3-D situations.

Several attempts have been made to do this already.

FLUENT/RELAP5

The Idaho National Engineering & Environmental Lab (INEEL) has begun a programme to couple its RELAP5-3D© advanced thermal-hydraulic systems analysis code to FLUENT. The code coupling will enable CFD-level analysis of critical components in an overall system model described by RELAP5-3D. Both steady-state and transient calculations can be performed using many working fluids and also point to three-dimensional neutronics. The FLUENT/RELAP5-3D coupled code is intended as a state-of-the-art tool to study the behaviour of systems with single-phase working fluids, such as advanced gas-cooled reactors. For systems with two-phase working fluids, particularly during LOCA scenarios where a multitude of flow regimes, heat transfer regimes, and phenomena are present, the FLUENT-RELAP5-3D coupling will have less general applicability since FLUENT's capabilities to analyse global two-phase problems remain limited. Consequently, for two-phase advanced reactor analysis, INEEL plans to employ not only the FLUENT-RELAP5-3D coupling, but also to make use of state-of-the-art experimental CFD tools such as CFDLib (available from the Los Alamos National Laboratory).

In a recent Swedish project, comparisons between two simulations using RELAP5/mod 3.2.2 gamma and RELAP5-3D mod 2.0 were made for heat in a feedwater pipe or steam line. The first 0.1 seconds of the transient was calculated. In both models, the pressure vessel upper part and the downcomer region (bounded by the core shroud) were modelled. The results showed only small effects of a full 3D simulation (CFD) compared to a simulation with a "mesh-like" (downcomer) and "gitter-like" model (above the core), using the traditional RELAP-5-technique with junctions. This was the result for the different test cases for a steam line break. However, considerable deviation in the results was found for the feedwater pipe breaks, which is believed to be due to some shortcomings in the numerics during the first few time steps for the version used (Ref. 3). The formal report (Ref. 4) is not yet issued. Comparisons between TRACE and RELAP-5 are also underway in the context of a new project.

In an internal development at GRS, the 1-D system code ATHLET has been dynamically coupled with the CFD code FLUBOX-3D, and used to analyse Test 6 from the UPTF series. This was done specifically to enable asymmetric flow in the downcomer to be captured as well as important motions in the lower plenum.

Thus, although the beginnings of a system-code/CFD-code coupling has appeared, considerably more effort is required to broaden the technique, and make it available to the general user. A related validation database containing non-proprietary information also needs to be assembled.

Ref. 1: R. R. Schultz, W. L. Weaver, *"Using the RELAP5-3D Advanced Systems Analysis Code with Commercial and Advanced CFD Software"*, Paper 36545, ICONE-11, Tokyo, Japan, April 20-23, 2003.

Ref. 2: U. Graf, "Zwei-dimensionale Berechnung einer Gegenströmung von Wasser und Dampf im Ringraum eine Reaktordruckbehälters mit ATHLET/FLUBOX, GRS-A-2419, Garching, 2001.

Ref. 3: M. Henriksson, personal communication with F. Alavyoon at Forsmark Kraftgrupp AB.

Ref. 4: H. Lindqvist, *"An example of comparisons between RELAP-5 and RELAP-5-3D-application to transients in a pressure vessel after a pipe break"*, Forsmark Kraftgrupp, FT-report (preliminary, to be issued).

5.2 Information on Transient Behaviour

Relevance of the phenomenon as far as NRS is concerned
In contrast to many other industrial applications of CFD, those relating to NRS often involve the simulation of transients, and often long transients.

What the issue is
Generally, there is a lack of data against which to validate time-dependent CFD calculations. Many of the tests arising from the nuclear area are integral in nature, and do not have the local data required to validate CFD models. In addition, transient simulations are often too burdensome for *Best Practice Guidelines* techniques to be strictly applied.

What the difficulty is and why CFD is needed
Integral tests have formed the backbone of nuclear safety philosophy for many years, and the experience has been accumulated in the correlations currently employed in (0-D) lumped-parameter and (1-D) system codes. Those situations requiring CFD analysis (and many such have been alluded to in this report) may bypass the knowledge embodied in established correlations, replacing it by a detailed local analysis, in order to develop basic understanding. This new approach requires careful application, and validation.

What has been attempted and achieved/what needs to be done (recommendations)
The ISP-43 exercise, based on boron dilution experiments carried out at the University of Maryland, has provided valuable CFD validation data of general relevance to single-phase mixing phenomena in reactor pressure vessels. Other exercises (MISTRA, TOSQAN, UPTF) provide bases for the development of two-phase CFD models. In addition, IAHR benchmarks (mixed convection, natural circulation, flow in tee-junctions) are a good source of general transient hydraulic data. However, the entire area of transient simulation and benchmarking needs to be brought into a common database.

Ref. 1: ISP-43: Rapid Boron Dilution Transient Experiment, Comparison Report, NEA/CSNI/R(2000)22.

Ref. 2: F.-P. Weiss *et al.*, *"Fluid Mixing and Flow Distribution in the Reactor Circuit (FLOWMIX-R)"*, Proc. FISA-2003/EU Research in Reactor Safety, 10-13 Nov. 2003, Luxembourg.

5.3 Range of Application of Turbulence Models

Relevance of the phenomenon as far as NRS is concerned
Almost exclusively, CFD simulations of NRS problems involve turbulent flow conditions.

What the issue is
The turbulence community has assembled and classified a large selection of generic flow situations (jets, plumes, flows though tee-junctions, swirling flow, etc.), and made recommendations of which turbulence models are most appropriate. Care is needed to ensure that in NRS applications the turbulence model has been chosen appropriately.

What the difficulty is
CFD is not capable of modelling entire reactor systems, which means that sections of the system must be isolated for CFD treatment. The range of scales can be large (e.g. in containments), and/or the flow phenomena rather special (e.g. ECC injection). It is necessary to extend the database of recognised flow configurations to include those particular to NRS applications of CFD, and build a suitable validation base.

What has been attempted and achieved/what needs to be done (recommendations)
A very good exposé of this issue is given in the ECORA BPGs, so only a sketch will be given here.

In most industrial applications of CFD, RANS models are employed. However, due to the averaging procedure, information is lost, which has then to be fed back into the equations via an appropriate turbulence model. The lowest level of turbulence models offering sufficient generality and flexibility are two-equation models. They are based on the description of the dominant length and time scale by two independent variables. More complex models have been developed, and offer more general platforms for the inclusion of physical effects. The most complex are Second Moment Closure (SMC) models. Here, instead of two equations for the two main turbulent scales, the solution of seven transport equations for the independent Reynolds stresses and one length (or related) scale is required.

The challenge for the user of a CFD method is to select the optimal model for the application at hand from the models available in the CFD method. It is not trivial to provide general rules and recommendations for the selection and use of turbulence models for complex applications. Two equation models offer a good compromise between complexity, accuracy and robustness. The most popular models are the standard k-ε model and different versions of the k-ω model. However, the latter shows a severe free-stream dependency, and is therefore not recommended for general flow simulations, as the results are strongly dependent on user input.

An important weakness of standard two-equation models is that they are insensitive to streamline curvature and system rotation. Particularly for swirling flows, this can lead to an over-prediction of turbulent mixing and to a strong decay of the core vortex. There are curvature correction models available, but they have not been generally validated for complex flows. On the other hand, SMC models are much less robust, and it is often recommended to perform a first simulation based on the k-ε model, and use this as a starting point for the SMC approach. However, such an approach is hardly feasible for transient simulations, which are usually required for NRS applications.

The amount of information to be provided by the turbulence model can be reduced if the large time and length scales of the turbulent motion are resolved explicitly. The equations for this so-called Large Eddy Simulation (LES) method are filtered over the grid size of the computational cells. All scales smaller than that provided by the resolution of the mesh are modelled, and all scales larger than the cells are computed. This approach is several orders of magnitude more expensive than a RANS simulation and is therefore not used routinely in industrial flow simulations.

However, for certain classes of applications, LES will be applicable in the near future. The most appropriate area will be free shear flows, where the large scales are of the order of the solution domain (or only an order of magnitude smaller). For boundary layer flows, the resolution requirements are much higher, as the near wall turbulent length scales become much smaller. Internal flows (pipe flows, channel flows) are in between, as they have a restricted domain in the wall normal direction, but small scales have to be resolved in the other two directions.

LES simulations do not easily lend themselves to the application of grid refinement studies, for either the time or space domains. The main reason is that the turbulence model adjusts itself to the resolution of the grid. Two simulations on different grids may not be compared by asymptotic expansion, as they are based on different levels of the eddy viscosity, and therefore on a different resolution of the turbulent scales. From a theoretical standpoint, the problem can be avoided if the LES model is not based on the grid spacing but on a pre-specified filter-width. This would allow grid-independent LES solutions to be obtained. However, LES remains a very expensive approach to turbulence modelling, and systematic grid and time step studies too prohibitive, even for a pre-specified filter. It is one of the disturbing facts that LES does not lend itself naturally to the application of BPGs.

Recently, there are moves to combine trustworthy correlations with CFD modelling [Refs. 2,3]. Care must be taken when doing this, since many correlations are built on bulk values of the relevant quantities (e.g. tangential velocities, temperatures), whereas a CFD treatment would probably need to rely on local variables, in order to maintain generality.

Ref. 1: Menter, F. *"CFD Best Practice Guidelines for CFD Code Validation for Reactor-Safety Applications"*, ECORA BPGs, 2002.

Ref. 2: Menter, F. *et al*. *"A Correlation-Based Transition Model using Local Variables. Part I: Model Formulation"*, Proc. ASME Turbo Expo 2004, Power for Land, Sea and Air, June 14-17, 2004, Vienna, Austria.

Ref. 3: Menter, F. *et al. "A Correlation-Based Transition Model using Local Variables. Part II: Test Cases and Industrial Applications"*, Proc. ASME Turbo Expo 2004, Power for Land, Sea and Air, June 14-17, 2004, Vienna, Austria.

5.4 Two-Phase Turbulence Models

This is a two-phase phenomenon, and is covered in detail in the WG3 document.

Orientation
Turbulence modelling seems to be presently limited to extrapolations of the single phase k-epsilon models by adding interfacial production terms. The limits of such approaches have already been reached, and multi-scale approaches are necessary to take account of the different nature of the turbulence produced in wall shear layers, and the turbulence produced in bubble wakes. Certainly, more research effort is required in this area.

5.5 Two-Phase Closure Laws in 3-D

This is a two-phase phenomenon, and is covered in detail in the WG3 document.

Orientation
Increasingly, the two-fluid (sometime three-fluid, to include a dispersed phase) model is being adopted for the multi-phase CFD simulations currently being carried out. In this approach, separate conservation equations are written for each phase. These equations require closure laws representing the exchange of mass, momentum and energy between the phases. Except for rather particular flow regimes (separated phases, dispersed second phase) genera-purpose expressions for such closure laws requires extensive further development.

5.6 Experimental Database for Two-Phase 3-D Closure Laws

This is a two-phase phenomenon, and is covered in detail in the WG3 document.

5.7 Stratification and Buoyancy Effects

Relevance of the phenomenon as far as NRS is concerned

Buoyancy forces develop in the case of heterogeneous density distributions in the flow. Most of the events concern thermally stratified flows, which result from differential heating (e.g. in heat exchangers), or from incomplete mixing of flows of different temperature (e.g. thermal stratification).

Other contributions to this report have underlined the possible occurrence of stratification and buoyancy forces. For single phase flows, one can recall stratified flow developing in the case of "hot leg heterogeneities (see Section 3.8), in the case of thermal shock (Section 3.12), induced break (Section 3.14), and for natural convection in many relevant safety situations for GFRs and LMFBRs in the context of PAHR (Post Accident Heat Removal); see specific Sections. For two-phase flow problems, the reader is referred to the WG3 document. Stratification may be one of the significant phenomena in the case of thermal shock, under some small-break LOCA conditions (see Section 3.22 on the AP600), and for waterhammer condensation. Stratification and buoyancy effects may lead to thermal fatigue, to modification of condensation rates, and to difficulties in predicting the associated mixing processes.

What the issue is

Stratified flows and buoyancy-induced effects take place in many parts of the flow circuit: main vessel, lower and upper plena, pipes, and hot and cold legs. Most of the time, the phenomena are associated with unsteady 3D flow situations. The issue is to derive a modelling strategy able to handle all the situations of relevance to NRS.

What the difficulty is and why CFD is needed

These complex phenomena are difficult to take into account using a system-code approach, and CFD is needed to better predict the time evolution of such flows, in particular the mixing rate between flows of different temperature (stratification may limit the action of turbulence, while buoyancy may in some cases promote mixing), and, in case of two phase flows, the behaviour of the different phases of the flow and the associated condensation rate.

For the case of single-phase flows, there remain difficulties and uncertainties concerning the modelling of turbulence for such situations. The standard k-epsilon model is known to poorly take into account mixing in strongly buoyant situations, and more complex closures (e.g. the Reynolds Stress Model) may be recommended for obtaining satisfactory results (Ref. 1). Unfortunately, the RSM model is much less robust that the k-epsilon model, and it may be difficult, or even impossible, to obtain converged solutions in complex geometries. Additionally, two further issues may be underlined: (i) the transitional state of such flows is difficult to handle in some situations, and (ii) the use of wall functions may lead to uncertainties if they are not designed for buoyant situations. (CFD two-phase flow issues are covered in the appropriate sections.)

What has been attempted and achieved/what needs to be done (recommendations)

Numerous CFD simulations have already been undertaken for specific situations, including the use of turbulence modelling, wall functions, etc. Due to the large number of the situations analysed, the main recommendation may concern the development of specific experiments to assess the validity range of the existing modelling capability.

Ref. 1: M. Casey, T. Wintergerste (Eds.), "ERCOFTAC Special Interest Group on Quality and Trust in Industrial CFD: Best Practice Guidelines, Version 1.0, January 2000.

5.8 Coupling of CFD code with Neutronics and Structure Codes

Neutronics

Relevance of the phenomenon as far as NRS is concerned
Precise prediction of the thermal loads to fuel rods, and of the main core behaviour, result from a balance between the thermal hydraulics and the neutronics.

What the issue is
Basic understanding consists of recognising that the thermal hydraulics is coupled with the neutronics through the heat release due to neutronic activity (nuclear power distribution and evolution), and that the neutronics is coupled with the thermal hydraulics through the temperature (fuel and moderator), density (moderator), and the possible concentration of neutron absorber material (e.g. boron, see Section 3.7).

What the difficulty is and why CFD is needed
The difficulty is to perform a coupled simulation, involving a CFD code adapted to the core description and a neutronics code, and to ensure consistent space and time precision of the two aspects.

What has been attempted and achieved/what needs to be done (recommendations)
Some progress has been made in this area.

The current state of the art is a coupling between a sub-channel description of the thermal hydraulics and neutron diffusion at the assembly level, for both steady-state and transient situations (c.f. OECD/NEA benchmarks). Pin or cell level coupling has also been investigated.

The coupling between a CFD code (Trio_U) and a Monte-Carlo neutronics code (MCNP) has been tested in the context of a PhD programme for the MSRE prototype. The results obtained so far compare well with the experimental data. Their extrapolation suggests ways of improving the safety coefficients of power molten-salt reactors (Ref. 1).

CFD neutronic coupling between STAR-CD and VSOP is proposed in the case of PBMR (see Ref. 2).

Coupling between core thermalhydraulics and neutronics with the SAPHYR system [Ref. 3] is based on the FLICA4 3D two-phase flow model and the CRONOS2 3D diffusion and transport models.

Several benchmarks have been computed in the frame of OECD/NEA [Ref. 4]: PWR Main Steam Line Break [Ref. 5], BWR Turbine Trip [Ref. 6], and currently the VVER-1000 Coolant Transient (for which fine-mesh CFD models are used). CRONOS2 and FLICA4 have also been successfully applied to the TMI Reactivity Insertion Accident benchmark (with BNL and KI, Refs 7-8], with pin-by-pin modelling, and within the NACUSP project (5th European FP, Ref. 9].

The 3D model of FLICA4 takes into account cross-flows between assemblies, related to core inlet boundary conditions or neutronic power distribution. Feedback parameters, such as fuel temperature and moderator density, are computed at the fuel assembly level, without collapsing several assemblies into macro-channels, which results in a better accuracy for local parameters of interest for safety: i.e. power peak and maximum fuel temperature. For conditions in which there is large asymmetry, like rod ejection or main steam-line break(SLB), FLICA4 features a two-level approach (zoom): the assembly level and the sub-channel level, either by coupling two FLICA4 calculations (exchange of boundary conditions), or by using a non-conforming mesh.

The coupling of another CFD code (CAST3M) with the neutronics code (CRONOS2) has been performed by CEA for the core of a gas-cooled reactor (GTMHR), in order to evaluate feedbacks (Ref.1 11). Similar work is being performed at Framatome, with the development of the coupling of the STAR-CD code with the CRONOS2 code.

Possible improvements would be (i) the coupling of CFD codes with more advanced (i.e. deterministic or stochastic transport) neutronics models; (ii) the development of a multi-scale approach, in order to optimise the level of description with the conditions, since, in many 3D cases, the power is very peaked (rod ejection, boron dilution, SLB, etc.), and fine-scale models could be used only in a limited region; and (iii) the development of time-step management procedures for complex transients in which the thermal hydraulics and neutronics time-scales are not the same.

Ref. 1: F. Perdu *"Contributions aux études de sûreté pour des filières innovantes de réacteurs nucléaires"*, PhD thesis, Université Joseph Fourier Grenoble, 2003.

Ref. 2: http://www.cd-adapco.com/news/18/reactor.htm.

Ref. 3: C. Fedon-Magnaud *et al.* *"SAPHYR: a code system from reactor design to reference calculations"*, M&C 2003 (ANS), Gattlinburg, Tennessee, April 6-11, 2003.

Ref. 4: http://www.nea.fr/html/science/egrsltb.

Ref. 5: E. Royer, E. Raimond, D. *Caruge "CEA-IPSN participation in the MSLB benchmark"*, Nuclear Technology, to be published.

Ref. 6: G. Mignot, E. Royer, B. Rameau, N. Todorova *"Computation of a BWR turbine trip with Cathare-Cronos2-Flica4 coupled codes"*, Nuclear Science and Engineering, to be published.

Ref. 7: P. Ferraresi, S. Aniel, E. Royer, *"Calculation of a reactivity initiated accident with a 3D cell-by-cell method: application of the SAPHYR system to the TMI1-REA benchmark"*, CSNI Workshop, Barcelona, April 2000.

Ref. 8: J.C. Le Pallec, E. Studer, E. Royer, "PWR Rod Ejection Accident: Uncertainty analysis on a high burn-up core configuration", Int. Conf. On Supercomputing in Nuclear Applications (SNA). Paris, 2003.

Ref. 9: K. Ketelaar *et al.* *"Natural Circulation and Stability Performance of BWRs (NACUSP)"*, FISA-2003, Luxembourg, November 10-13, 2003.

Ref. 10: E. Studer *et al.*, *"Gas-Cooled Reactor Thermal-Hydraulics using CAST3M and CRONOS2 codes"*, Proc. 10th Int. Topical Meeting on Nuclear Thermal-Hydraulics, NURETH-10, Seoul, Korea, October 5-9, 2003.

Structures

Relevance of the phenomenon as far as NRS is concerned

The flows in the primary circuit components of reactors are often strong enough to induce vibrations in, or damage to, confining or nearby structures, which may have consequences regarding plant safety. In the case of thermal-hydraulic issues relating to the containment, both the flow inside the containment volume, and the heat transfer to the walls, have to be simulated simultaneously, usually by coupling implicitly a CFD code and structure code.

What the issue is

In order to obtain detailed information on the thermal and/or pressure loads to the structures, CFD analysis of the flow field is often necessary. To facilitate the transfer of the load information, it is often desirable, and sometimes necessary, to directly link CFD and structure codes. If there is no feed-back of structural displacement on the flow field, it is sufficient to have a one-way coupling only, and the structural analysis can be performed "off-line" to the CFD simulation. However, if there is a feed-back, for example due to changes in flow geometry, a two-way coupling between the codes is needed, and the CFD and structural analysis must be computed simultaneously (or perhaps just iteratively in simple cases).

What the difficulty is and why CFD is needed

The pressure loading to structures may be computed at different levels of sophistication. In simple cases, a static loading, estimated using lumped-parameter methods, may be input as a boundary condition to the stress analysis program. Similarly with thermal loading, provided a reliable estimate of the heat transfer coefficient may be given. In these circumstances, the stress analysis may be performed independently of any associated CFD. However, if there are significant spatial variations in the loadings, it may be necessary to provide cell-by-cell information of the flow details. CFD is needed for this.

What has been attempted and achieved/what needs to be done (recommendations)

The code coupling of the structural mechanics code ANSYS and the CFD code CFX has been applied for different aerodynamic test cases (Ref. 1). The analysis of a pitching airfoil demonstrates the performance of CFX for the prediction of the transient lift and momentum coefficients. Furthermore, the mechanical coupling example of an elastic-walled tube shows the flexible coupling concept between structural and fluid software. The combination of both, transient and flexible coupling is applied for the AGARD 445.6 wing flutter test. A good agreement has been obtained for the comparison of the flutter frequency in a wide range of Mach numbers. The technology for NRS-related issues, e.g. flow-induced vibrations, water-hammer, etc., would follow similar lines.

Coupling between STAR-CD and Permas is described on the website http://www.cd-adapco.com/news/16/fsiinnotec.htm). The deformations and stresses of the Sulzer Mixer, subjected to high-pressure load, was investigated by coupling STAR-CD and Permas using MpCCI. The geometry model takes into account all the details of the structure, even welding points. The mixer structure was built entirely as a 3D solid model using Unigraphics. As a first step, the steady-state fluid flow was computed by STAR-CD without any code coupling. As a second step, the fluid forces were transferred from the fluid code to the stress code by coupling the codes. This method (one-way-coupling) assumes that the fluid flow topology is not affected by the displacement of the mixer. This is realistic for the kind of mixer under consideration, and would be true also for many NRS applications involving heavy reactor components. The deformations, stresses and rotational movement agreed with experimental observations. Work on the full coupling of the flow and stress computations, requiring STAR-CD's moving-mesh capability, is in progress. The use of STAR-CD, Permas and MpCCI provides more realistic computation of the forces on the structures, and better design and optimisation of the mixer geometry.

Recently, a link has been established between the CFD code FLUENT and the structures code ABAQUS. In summary, the effect of a flow field on a deformable solid is computed using a coupled solution technique. Hydrodynamic pressure is computed in FLUENT and exported to ABAQUS, where its impact on the solid is calculated. The easy transfer of data between the packages suggests that the method can and should be applied to more complex scenarios that involve more complicated geometries and/or physics, such as those arising in NRS. At present, the coupling between the codes is one-way only.

Prof. F. Grosjean and his student, S. Sauvage, at ENSIETA in France have validated an iterative approach to modelling fluid-structure interaction. Their study, presented at the 1998 ABAQUS Users' Conference, examines the deformation of a thin aluminium slab in a cross-flow of air by coupling a FLUENT simulation of the airflow to an ABAQUS prediction of the structural deformation. Starting with a prediction of air flow around the non-deformed slab, the researchers determined the pressure forces on the slab, and used these as input to ABAQUS. The ABAQUS calculations predicted the slab deformation, which was used to redefine the FLUENT mesh defining the flow geometry. Using the modified mesh, the FLUENT calculations predicted new pressure forces as modified inputs to the ABAQUS run. By iterating between the two codes, the ENSIETA team converged to a steady-state prediction of the flow around the deformed slab. The calculation procedure was validated against wind tunnel test data on deformation and drag. Calculations were within about 3% of measurements for both quantities. Again, this technique has potential application to many NRS issues involving fluid-structure interaction.

CEA has made a study of the mechanisms leading to cracking in mixing zones of piping networks, as a result of thermal loading. The overall analysis was performed with a single computer code: the CAST3M code developed by CEA. Cracks appearing in a mixing tee, and its connection with the pipework in the Civaux Unit 1, were adequately explained by the various calculations made.

A run-time coupling using PVM (Parallel Virtual Machine) has been established between the codes COCOSYS (a lumped-parameter containment code) and CFX. The aim of the work was to replace certain user-specified locations of the domain described by COCOSYS by a CFX model, and to exchange the boundary fluxes of mass and energy between the codes on-line. Because COCOSYS solves only a simplified set of equations, neglecting conservation of momentum, in some situations for which momentum dominates, it may be that CFX would provide much better predictions. Specific locations in the containment, identified before the calculation begins to be candidates for higher flow speeds or strong gas gradients, can be replaced by an appropriate CFX model with a pre-prepared grid. COCOSYS has the general control of the calculation, and the CFX simulation is started at the specified time. The CFX results are then used for the region covered. The data exchange starts by communicating initial data to CFX, and later by sending back to COCOSYS the flows across the boundaries. PVM serves as the transport paradigm, and provides all necessary routines for any data transfer. So far, the coupling between COCOSYS and CFX has been realised for mass and energy flow through openings, and heat transfer through walls without mass exchange.

Ref. 1: Kuntz, M., Menter, F.R., *“Simulation of Fluid Structure Interaction in Aeronautical Applications”*, to be published in the ECCOMAS 2004 Conference, July 2004.

5.9 Coupling CFD with System Codes: Porous Medium Approach

FLUBOX/ATHLET

Thermal-hydraulic system codes for fluid flow simulation in nuclear power plants, *e.g.* the ATHLET code [2,3], consist of a network of one-dimensional objects. These objects simulate pipes, pumps, pressurisers, the lower plenum, the reactor core, etc. Each component, and consequently the entire power plant facility, can be assembled from these basic objects. In situations where multi-dimensional effects become important, multi-dimensional objects must be added to this component network. The multi-dimensional object could, in principle, be any multiphase CFD code.

The coupling of multidimensional objects with the one-dimensional network of a system code consists of mainly three tasks.

- The first task is to exchange the relevant data shared by the two systems. For this one needs an interface for the data exchange between the differently structured programs. The possibility of different spatial discretisations must also be considered here (e.g. staggered or non-staggered grids).

- The second task is the physical coupling. The programs may use different physical models for the simulation of the fluid flow (e.g. in two-phase flow the models range from homogeneous models to fully separated two-fluid models). Another problem is the different spatial dimension (1-D and multi-D) of the approximation. Depending upon the engineering configuration, reasonable connections must be established between the technical components represented by different spatial approximation.

- The successful execution of the first two tasks leads to an *explicit* coupling of the program systems.

- The third task is the efficient solution of the coupled system. The coupled system must be solved implicitly in time, otherwise it will suffer from Courant limit restrictions. The problem size of the combined system is the sum of the problem sizes of the separate systems, and the matrix of the linear system of the combined problem is accordingly upsized. Hence, much larger linear systems of equations than that of the separate systems must be solved.

- In a prototype coupling of the system code ATHLET and the CFD code FLUBOX it was shown how the two programs can be coupled in an efficient way [1], where the solution process of the implicitly coupled combined system maintains the solution methods for each separate system. The process of the implicit coupling is performed by a fractional step method.

Ref. 1: U.Graf, Implicit Coupling of Fluid-Dynamic Systems: Application to Multidimensional Countercurrent Two-Phase Flow of Water and Steam, *Nuclear Science and Engineering*, 129, pp 305-310, 1998

Ref. 2: V.Teschendorff, H.Austregesilo, G.Lerchl, Status and plans for development and assessment of the code ATHLET. *Proceedings of OECD/CSNI Workshop on Transient Thermal-Hydraulic and Neutronic Codes Requirements*, NEA/CSNI/R (97)4, pp.112,Annapolis, USA, Nov. 5-8, 1996.

Ref. 3: V.Teschendorff *et al.*, ATHLET Home Page, http://www.grs.de/en/working_fields/reactor_safety/transients_leakages/athlet.html.

5.10 Computing Power Limitations

The original version of *Parkinson's Law* [1], "Work expands to fill the time available", was first articulated by Prof. C. Northcote Parkinson in his book of the same name, and is based on an extensive study of the British Civil Service. The scientific observations which contributed to the law's development included noting that as Britain's overseas empire declined in importance, the number of employees at the Colonial Office increased. From this have arisen a number of variants. Two pertinent ones from the sphere of information technology are: *Parkinson's Law of Data*, "Data expands to fill the space available for storage", and *Parkinson's Law of Bandwidth Absorption*, "Network traffic expands to fill the available bandwidth". The application of CFD methodology also deserves a mention. Perhaps *Parkinson's Law of Computational Fluid Dynamics* could read: "The number of meshes expands to fill the available machine capacity".

Despite the overwhelming amount of possibilities and advantages of present CFD codes, their role should not be exaggerated. The development of codes able to compute LOCA phenomena with some realism began in the 1970s, which, by modern standards, was a period of very limited computing power. Typically, good turn-round could only be achieved using supercomputers. Today, these system codes are recognised internationally. The physical models are based on reasonable assumptions concerning the steam and water flows, and their interaction. The circuits are treated as an assembly of 1D pipe elements, 0D volumes, and eventually some 3D component modelling. Intensive experimental programs of validation on system loops, or local component mock-ups, were carried out. So there is some confidence in their results, provided they are used in their domain of validation, and by experienced users.

Today, a large part of the system calculations are made on workstations or PCs. In the mid-term, say 5 to 10 years, it is foreseen to improve the two-fluid models, perhaps with extension to three fields to include droplets and bubbles, and incorporation of transport equations for interfacial area; 3D modelling would be used, as required. During the same period, the increasing computer efficiency will allow the use of refined nodalisation, and the capture of smaller scale phenomena, provided more sophisticated models are available. Certainly, with the time needed for validation programmes, the development of modelling sophistication will not keep pace with the upgrades in computer performance. It is unlikely then, that system-code NRS analyses will ever again require super-computing power.

However, even with the advances in computer technology, it is difficult to see CFD codes being capable of simulating the whole primary or secondary loop of a nuclear plant: system and component codes will still remain the main tools for this. However, for those occasions when CFD is needed – and many examples of this have been given in this document – the computations will stretch computing resources to the limit, just as predicted by Parkinson’s Law.

The CFD codes will allow the zooming in on specific zones of a circuit, or may be used as a tool to derive new closure relations for more macroscopic approaches, reducing the necessity of expensive experimental programmes. Coupling between CFD and system codes may also be an efficient way to improve the description of small-scale phenomena, while living within current computer limitations. As soon as in-progress developments are available, Direct Numerical Simulation (DNS) codes will be used for a better understanding of small-scale physical processes, and for the derivation of new models for averaged approaches.

These days, CFD simulations using 10 000 000 meshes are common in many industrial applications. Such computations are possible because invariably the calculations are steady-state, single-phase, and carried out using parallel-architecture machines. In NRS applications, many of the situations requiring analysis are of a transient nature. CFD codes are computationally demanding, both in terms of memory usage and in the number of operations. Since the accuracy of a solution can be improved by refining the mesh, and by shortening the time step, there is a tendency to use whatever computational resources are available, and there is a never-ending and never-compromising demand for faster machines, and more memory – Parkinson’s Law again!.

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, remain 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. Typically, the number of iterations M to convergence within a time step is also proportional to N. Thus finally, the run-time for the CFD code should scale according to

$$t \propto N^5$$

where the constant of proportionality, among other things, depends linearly on the total simulation time – and simulation times in NRS applications can be very long.

Despite the continual improvement in processor power, the commodity computer market has still not overtaken the demands of CFD. Traditionally, programs were written to run on a single processor in a serial manner, with one operation occurring after the next. 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. Since 1990, the use of parallel computation has shifted from being a marginal research activity to the mainstream of numerical computing.

A recent study [3] has shown that the scaling up of performance with 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. The speed of a program also depends on the language (generally, Fortran is faster than C), the compiler (levels of optimisation), and the syntax used to express basic operations (machine-dependent). With regards to the syntax of operations, forms that are fast on one platform might be slow on another. Modern workstations have proved to give good performance for small array sizes that fit into the processor's cache. However, when the array is too large to fit into the cache, the speed of the computers can drop to half their peak performance. These machines commonly bank their memory, and array sizes which result in the same memory bank being accessed multiple times for the one operation will incur a performance penalty as a result. This problem can commonly be solved by increasing the leading dimension of an array.

Vector computers have an optimum speed when the array dimensions are a multiple of the size of the vector registers, typically a multiple of 8. Thus, when comparing a vector computer to a workstation, the optimum array size for the vector platform is the slowest (due to memory banking) on the workstation. Shared memory parallel computers typically give good performance for small to moderate problem sizes, for which the data fits within the cache of the computer's processors, but if array sizes are too large for the data to fit into the cache, there is a severe drop in speed, as all processors attempt to access the shared memory. In comparison, it was found [3] that distributed memory machines achieved poor speeds for small to moderate array sizes, whereas for large problems, for which the memory access speed rather than inter-processor communication speed dominated, the parallel paths to memory ensured a near linear speedup with number of processors.

Given this linear speedup, and the N^5 dependence of runtime on number of meshes in one coordinate direction, doubling the number of processors, and keeping total runtime the same, the number of meshes in each direction can be increased by about 15%, say from 100 to 115. 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 32.

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 some years to come. In the mid-term, compromises will have to be made: for example, examining mesh sensitivity for a restricted part of the computational domain, or to a specific period in the entire transient. Certainly, expanding efforts in NRS will ensure that Parkinson's Law will prevail for CFD.

Ref. 1: C. Northcote Parkinson, *Parkinson's Law: The Pursuit of Progress*, London, John Murray (1958).

Ref. 2: M. Livolant, M. Durin, J.-C. Micaeli, *"Supercomputing and Nuclear Safety"*, Int. Conf. on Supercomputing in Nuclear Applications, SNA'2003, Paris, Sept. 22-24, 2003.

Ref. 3: S. E. Norris, *"A Parallel Navier-Stokes Solver for Natural Convection and Free-Surface Flow"*, Ch. 6, PhD Thesis, Dept. Mech. Eng., University of Sydney, Sept. 2000.

5.11 Special Considerations for Liquid Metals

Relevance of the phenomena as far as NRS is concerned

The conventional fast breeder reactor uses liquid metal, such as Na, NaK or Pb etc., as coolant. The following liquid-metal hydraulics phenomena are relevant as far as NRS is concerned: (i) natural convection, (ii) thermal striping, (iii) sloshing of free surface, (iv) sodium fires, and (v) sodium boiling. It seems that some established CFD studies have been carried out concerning natural convection and sodium fires; these are described in Section 3.22 of this report. Identification of gaps in the technology base for special considerations for liquid metals, therefore, is restricted to thermal striping, sloshing of the free surface and sodium boiling.

What the issue is

Thermal striping phenomena in LMFBRs, characterised by stationary, random temperature fluctuations, are typically observed in the region immediately above the core exit, and are due to the interaction of cold sodium flowing out of a control rod assembly and hot sodium flowing out of adjacent fuel assemblies. The same phenomenon occurs at a mixing tee, a combining junction pipe, etc. The temperature fluctuations induce high-cycle fatigue in the structures.

The sodium in the reactor vessel has a free surface, and is covered by an inert gas. When the reactor vessel is shaken by seismic forces, waves will form on the free surface: the so-called "sloshing behaviour". If the amplitude of the wave increases, the inert gas may enter an inlet nozzle and be carried around the primary circuit, resulting in the formation of gas bubbles in the core region, causing a positive reactivity insertion. Another issue is the fluid force associated with slug movement caused by violent sloshing. The vessel wall and internal structures of LMFBRs are relatively thin, and mitigate thermal stress attributed to temperature variations during operation, which is characteristic of the high conductivity of liquid sodium. The fluid force of a moving liquid slug, therefore, could threaten the integrity of the reactor vessel.

Sodium boiling in the core region of LMFBRs would cause a power excursion, through feedback of positive reactivity coefficient of sodium void.

What the difficulty is and why CFD is needed to solve it

The design study associated with the protection of the Japanese LMFBR MONJU from thermal striping was performed using experimental data from a 1/1 scale model with sodium. In such a conventional approach, an increase in costs, as well as the time to perform the experiments, is inevitable, because it is technically difficult to obtain adequate amounts of quality of data from sodium experiments. CFD is needed to overcome this difficulty.

Linear-wave theory is applicable only to small-amplitude waves at the free surface. CFD is needed to solve the (non-linear) violent sloshing phenomenon important for NRS.

High accuracy is required from the sodium-boiling model, whose function is first to predict the exact time and location of the onset of boiling, and then to describe the possible progression to dryout. CFD has the potential to improve the accuracy in prediction of these phenomena.

What has been attempted and achieved / what needs to be done (recommendations)

The IAEA coordinated a benchmark exercise with the goal of simulating an accident in which thermal striping had caused a crack in a secondary pipe of the French LMFBR Phenix. JNC has been developing a simulation system for the thermal striping phenomena consisting of two CFD codes: AQUA and DINUS-3. AQUA is a 3D model for porous media with a RANS turbulent model, and DINUS-3 is a 3D model for open medium, with a DNS turbulent model (see Ref. 1).

There are two approaches being used to simulate free surface flows numerically. One assumes potential flow conditions, in which the basic equations to be solved are the Bernoulli equation with a velocity potential, the kinematical equation of the liquid surface, and the mass conservation equation of the liquid (see Ref. 2). The other uses a commercial CFD code that incorporates the VOF interface-tracking technique (see Ref. 3).

Numerous out-of-pile and in-pile experiments have been conducted to obtain information on sodium boiling, because in the past the power excursion scenario due to positive feedback of sodium void received the most attention by the LMFBR safety community. Whole-core accident analysis codes, such as SAS4A (see Ref. 4), have been developed for this purpose: they use a one-dimensional approach for the sodium-boiling module.

Ref. 1: T. Muramatu et al., "Validation of Fast Reactor Thermomechanical and Thermohydraulic Codes", Final report of a coordinated research project 1996-1999, IAEA-TECDOC-1318, 2002.

Ref. 2: M. Takakuwa et al., "Three-Dimensional Analysis Method for Sloshing Behavior of Fast Breeder Reactor and its Application to Uni-vessel Type and Multi-vessel Type FBR", Proc. Int. Conf. on Fast Reactors and Related Fuel Cycles, Vol. I, Oct. 28-Nov. 1, 1991, Kyoto, Japan.

Ref. 3: Seong-O. Kim et al., "An Analysis Methodology of Free Surface Behavior in the KALIMER Hot Pool", Proc. Third Korea-Japan Symposium on Nuclear Thermal Hydraulics and Safety, Oct. 13-16, 2002, Kyeongju, Korea.

Ref. 4: H.U. Wider et al., "Status and validation of the SAS4A accident code system", Proc. Int. Topical Meeting on LMFBR Safety and Related Design and Operational Aspects, Vol. II, p.2-13, Lyon, 1982.

5.12 Scaling

According to Wulff (1996), the purpose of scaling analyses is to provide:

1. the design parameters for reduced-size test facilities;

2. the conditions for operating experiments, such that at least the dominant phenomena taking place in the full-size plant are reproduced in the experimental facility over the range of plant conditions;

3. the non-dimensional parameters that facilitate the efficient and compact presentation and correlation of experimental results, which, by virtue of similarity and the parameter selection, apply to many systems, including both the test facility and the full size plant;

4. to identify the dominant processes, events, and characteristics (properties), all called here collectively "phenomena", to substantiate quantitatively, or revise, the expert-opinion-based, still subjective, ranking of phenomena in the order of their importance, i.e. the ranking which is normally arranged in the Phenomena Identification and Ranking Table (PIRT);

5. to select among all the available test facilities the one that produces optimal similarity and the smallest scale distortion, and to establish thereby the test matrix;

6. to provide the basis for quantifying scale distortions; and

7. to derive the scaling criteria, or simulating component interactions, within a system from the global component and system models, with the focus on systems, rather than component scaling.

In the context of CFD code assessments and code applications, items 4 and 5 are the most relevant. Moreover, at least one more item could be added to the list:

8. to help in transfer of knowledge acquired in validation of the code on scaled-down models to the simulation of a real industrial problem (e.g. to estimate the required grid size).

Traditional scaling analyses embody first normalising the conservation equations on the subsystem or component level for the test section, then repeating this subsystem level scaling for all the components in the system, and collecting all the local scaling criteria into a set of system scaling criteria. The claim is then made that the dynamic component interaction and the global system response should be scaled successfully with the set of criteria for local component scaling, because the system is the sum of its components. This principle applies only if all the local criteria are met, and complete similitude exists. Complete similitude, however, is physically impossible, because all scaling requirements cannot be met simultaneously for a system in which areas and volumes and, therefore, area-dependent transfer rates and volume-dependent capacities scale with different powers of the length parameter, and thereby produce conflicting scaling requirements.

Scaling groups can be derived using several methods, but two fundamental principles of scaling must be met (Wulff, 1996):

1. the governing equations are normalised such that the normalised variables and their derivatives with respect to normalised time and space coordinates are of order unity, and the magnitude of the normalised conservation equation is measured by its normalising, constant coefficient;

2. the governing equations are then scaled by division through the coefficient of the driving term; this renders the driving term of order unity, and yields fewer non-dimensional scaling groups, which measure the magnitudes of their respective terms, and therewith the importance of the associated transfer processes, relative to the driving term.

A categorisation of scaling approaches can be found e.g. in Yadigaroglu, Zeller (1994).

I. The simplest scaling technique is *linear scaling*, in which all length ratios are preserved: the mass, momentum and energy equations of a system, along which the equation of state, are non-dimensionalised, and scaling criteria are then derived from the resulting parameters; linear scaling leads to time distortion.

II. *Volumetric or time-preserving scaling* is another frequently used technique, also based on scaling parameters coming from the non-dimensionalised conservation equations; models scaled by this technique preserve the flow lengths, while areas, volumes, flow rates and power are reduced proportionally.

III. *Time-distorted scaling* criteria, described e.g. in Ishii, Kataoka (1984), include both linear and volumetric scaling as special cases, see Kiang (1985).

IV. A “structured” scaling methodology, referred to as *hierarchical two-tiered scaling* (H2TS), and proposed by Zuber (see e.g. Zuber, 1999), addresses the scaling issues in two tiers: a top-down (inductive) system approach, followed by a bottom-up, process-and-phenomena approach, since traditional local and component-level scaling cannot produce the scaling criteria for component interaction.

The last approach is described *e.g.* also in Zuber et al. (1998) and Wulff (1996), but its principles and procedures can be best made clear by its application to design of the APEX test facility (Advanced Plant

Experiment, Oregon State University), see Reyes, Hochreiter (1998). A short summary of their analysis follows.

The objective of this scaling study was to obtain the physical dimensions of a test facility that would simulate the flow and heat transfer during an AP600 Small Break LOCA. The APEX scaling analysis was divided into four modes of operation, each corresponding to a different phase of the SBLOCA:

3. closed loop natural circulation;
4. open system depressurisation;
5. venting, draining and injection;
6. long-term recirculation.

For each mode of AP600 safety system operation, the following specific scaling objectives were met:

7. the similarity groups, which should be preserved between the test facility and the full-scale prototype, were obtained;
8. the priorities for preserving the similarity groups were established;
9. the important processes were identified and addressed;
10. the dimensions for the test facility design, including the critical attributes, were specified; and
11. the facility biases due to scaling distortions were quantified.

To achieve this, eight tasks had to be performed during the scaling analyses.

1. To specify experimental objectives.
2. To prepare the SBLOCA Plausible Phenomena **I**dentification and Ranking Tables (PPIRTs) for each of the phases of a typical SBLOCA transient. Existing data on standard PWRs, coupled with engineering judgment and calculations for the AP600, were used to determine which SBLOCA thermal hydraulic phenomena might impact core liquid inventory or fuel peak clad temperature.
3. H2TS analysis for each phase of the SBLOCA was performed. The four basic elements of the H2TS method are:
    - *System subdivision*. The AP600 was subdivided into two major systems: a reactor coolant system and a passive safety system. These systems were further subdivided into interacting subsystems (or modules), which were further subdivided into interacting phases (liquid, vapour or solid). Each phase was characterised by one or more geometrical configurations, and each geometrical configuration was described by one or more field equations (mass, energy and momentum conservation equations).
    - *Scale identification*. The scaling level (system level, subsystem level, component level, constituent level) depending on the type of phenomena being considered was identified. A set of control volume balance equations was written for each hierarchical level.

- *Top-down scaling analysis*. For each hierarchical level, the governing control volume balance equations were written and expressed in dimensionless form by specifying dimensionless groups in terms of the constant initial and boundary conditions. Numerical estimates of the characteristic time ratios, Π_k, were obtained for the prototype and the model for each phase of the transient at each hierarchical level of interest. Physically, each characteristic time ratio is composed of a specific frequency, ω_k, which is an attribute of the specific process, and the residence time constant, τ_k, for the control volume. The specific frequency defines the mass, momentum or energy transfer rate for a particular process. The residence time defines the total time available for the transfer process to occur within the control volume. If $\Pi_k \ll 1$, only a small amount of the conserved property would be transferred in the limited time available for the specific process to evolve, and the specific process would not be important to the phase of the transient being considered. On the other hand, if $\Pi_k \geq 1$, the specific process evolves at a high enough rate to permit significant amounts of the conserved property to be transferred during the time period τ_k.

- *Bottom-up scaling analysis*. This analysis provided closure relations for the characteristic time ratios. The closure relations consisted of models or correlations for specific processes. These closure relations were used to develop the final form of the scaling criteria for purposes of scaling the individual processes of importance to system behaviour.

4. The scaling criteria were developed by setting the characteristic time ratios for the dominant processes in the AP600 to those for APEX at each hierarchical level.

5. The effect of a distortion in APEX for a specific process was quantified by means of a distortion factor DF, which physically represents the fractional difference in the amount of conserved property transferred through the evolution of a specific process in the prototype to the amount of conserved property transferred through the same process in the model during their respective residence times. A distortion factor of zero means that the model ideally simulates the specific process.

6. System design specification. The outcome of the scaling analysis was therefore a set of characteristic time ratios (dimensionless Π groups) and similarity criteria for each mode of operation. These scaling criteria were expressed in terms of ratios of model to prototype fluid properties, material properties, and geometrical properties. Now, working fluid, component materials, operating pressure, and the length, diameter and time scales can be selected.

7. Evaluation of key T/H PPIRT processes to prioritise system design specification.

8. APEX test facility design specifications and Q/A critical attributes.

The subject of scaling is very broad and cannot be dealt with in depth in this document. For CFD applications to NRS, it is comforting that, in principle, the computational model can be at 1-1 scale, but it remains important to ensure that the fluid-dynamic phenomena of relevance, validated against scaled experiments, have been preserved. This may be difficult if the fluid behaviour is categorised by flow-regime maps.

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6. METHODOLOGY FOR EXTENDING ASSESSMENT BASE

6.1 Evidence in support of CFD being classified as a proven technology

Validation Tests Performed by Major CFD Code Vendors

The code vendors identified here are those who promote general-purpose CFD: namely, CFX, STAR-CD, FLUENT and PHOENICS, all of whom have customers in the nuclear industry area. Other organisations with specialisations in certain areas, such as the aerospace industry, are excluded from the list, though those codes written specifically for nuclear applications, though not always available for general use, are included.

Each of the vendors operate in a commercial environment, and are keenly aware of their major competitors. Consequently, such a sensitive item as validation, which might lead them into an unwelcome code-code comparison exercise, may not receive all the attention it deserves. In addition, a validation activity may have been performed at the request of a particular customer, and the results restricted, or may not be published unless successful. Nonetheless, the companies are becoming more open, and have actively participated in international projects; the EU 5th Framework Programme ECORA is such an example.

The best source of information on specific validation databases is through the respective websites"

CFX	www.ansys.com
STAR-CD	www.cd-adapco.com
FLUENT	www.fluent.com
PHOENIX	www.cham.co.uk

Here one finds documentation, access to the workshops organised by each company, and to conferences and journal articles where customers and/or staff have published validation material. The most comprehensive documentation list appears to have been put together for PHOENICS, where a list of over 950 published papers can be found (some are validation cases), a special section devoted to validation issues is included on the website, and the code has its own journal containing peer-reviewed articles.

Clearly, the list of validation documents is too long to be written here, but evidence of its existence does confirm that commercial CFD has a well-founded technology base. It should be noted, however, that even for codes explicitly written for the nuclear community normally include basic (often academic) validation cases, just like those codes from the commercial area. A survey of validation tests has been put together by Freitas (Ref. 1).

Ref. 1 C.J. Freitas *"Perspective - Selected benchmarks from commercial CFD codes"* J. Fluids Engg. 117, 208.

GASFLOW

The GASFLOW code, which has been developed as a cooperation between Los Alamos National Laboratory (LANL) and Forschungszentrum Karlsruhe (FZK), is a 3D fluid dynamics field code used to analyse flow phenomena such as circulation patterns, stratification, hydrogen distribution, combustion and flame propagation, local condensation and evaporation phenomena, and aerosol entrainment, transport and deposition in reactor containments. GASFLOW is a finite-volume code, and based on robust numerical techniques for solving the compressible Navier-Stokes equations in Cartesian or cylindrical geometries. A semi-implicit solver is employed to allow large time steps. The code can model geometrically complex facilities with multiple compartments and internal structures, and has transport equations for multiple gas species, liquid water droplets, and total fluid internal energy. A built-in library contains the properties of 23 gas species and liquid water. GASFLOW can simulate the effects of two-phase dynamics with the homogeneous equilibrium model, two-phase heat transfer to and from walls and internal structures, catalytic hydrogen recombination and combustion processes, and fluid turbulence.

Ref. 1: J.R. Travis, J.W. Spore, P. Royl, K.L. Lam, T.L. Wilson, C. Müller, G.A. Necker, B.D. Nichols, R. Redlinger, *"GASFLOW: A Computational Fluid Dynamics Code for Gases, Aerosols, and Combustion"*, Vol. I, Theory and Computational Model, Reports FZKA- 5994, LA-13357-M (1998).

Ref 2: J.W. Spore, J.R. Travis, P. Royl, K.L. Lam, T.L. Wilson, C. Müller, G.A. Necker, B.D. Nichols, *"GASFLOW: A Computational Fluid Dynamics Code for Gases, Aerosols, and Combustion"*, Vol. II, User's Manual, Reports FZKA-5994, LA-13357-M (1998).

STAR-CD

Some elements relevant of the STAR-CD validation process are listed here: they derive from Workshop or University researches and are not nuclear oriented. CD Adapco, the company who market STAR-CD in Europe, is compiling a much more comprehensive validation list (including testing of turbulence models, heat transfer, multiphase flows, combustion,…), but the information is mainly derived from industrial cases, which are confidential. Consequently, it will not be available to this group.

Lid-Driven Cavity Flow

The problem is characterised by its elliptic and non-linear nature: numerical diffusion is tested. This study is concentrated on using the test case to compare the performance of the code with different types of mesh. Three types of mesh are used in this calculation, namely hexahedral cells, tetrahedral cells and polyhedral (trimmed) cells.

Two-Dimensional Single Hill Flow

This is one of the two test cases prepared for the ERCOFTAC Workshop on Databases and Testing of Calculation Methods for Turbulent Flows (organised as part of the 4th ERCOFTAC/IAHR Workshop on Refined Flow Modelling. Experimental data have been provided, and the main objective of the exercise was to demonstrate the accuracy of prediction attainable. This study is concerned with the turbulent flow past a surface mounted obstacle in a channel.

Supersonic Flow Over Flat Plate

This example concerns the development of the turbulent boundary layer on a two-dimensional wedge. The cross-sectional geometry of the wedge is an elongated trapezium with the top and bottom surfaces parallel. The leading edge is the intersection between the wedge's front and top surfaces, and the inclined angle between them is 6.7^o. The rear end of the wedge is vertical. Measuring from the tip of the leading edge to the trailing edge, the length of the wedge is 0.914 m. In the parallel part of the wedge, the thickness is 0.033 m.

During wind-tunnel tests, the flat surface of the wedge was kept parallel to the flow direction and hence at zero pressure-gradient. The model was placed in the centre of the working section, and the flow was considered to be two-dimensional. The wedge was not actively cooled, but was allowed to reach equilibrium temperature. Based on free-stream flow conditions of air, the Reynolds number was 15 350 000.

Turbulent Flow Over a Surface Mounted Rib

This study is concerned with turbulent flow past a surface-mounted obstacle in a channel. The obstacle, representing a fence or rib, spans the whole width of the channel. Tests were performed in air at 20^{o}C and over a range of flow velocities. Based on the mean inlet velocity and obstacle height, the Reynolds numbers ranged between 1500 to 3000.

Turbulent Vortex-Shedding around a Square Cross-Section Cylinder

This study is concerned with turbulent flow past a square-section cylinder, which exhibits natural periodic shedding of vortices. The experimental measurements were made by Durao et al. and the experimental configuration comprised a square cross-section cylinder spanning the whole width of a rectangular cross-section channel. According to their findings, the width of the test section was sufficiently large for the flow to be assumed two-dimensional at the central plane. Based on the mean flow velocity of water at inlet and on the height of the square, the Reynolds number was 14 000.

One-Dimension SOD's Shock Tube

A shock tube is simply a tube that is divided by a membrane or diaphragm into two chambers at different pressures. When the membrane is suddenly removed (broken), a wave motion is set up. This problem is characterised by the interface between the low and high-pressure chambers. The contact face, as it is known, marks the boundary between the fluids that were initially on either side of the diaphragm.

The main purpose of this validation case is to demonstrate the use of the gradient-based second order accurate differencing scheme (MARS) and the second-order temporal discretisation scheme in capturing the wave structures and motions.

Friction Factor of Fully Developed Turbulent Pipe Flow

The case of turbulent flow through pipes has been investigated thoroughly in the past, and a large amount of experimental data is available in the open literature. Because of its wide range of applications, it is also important for any CFD code to predict friction values that are comparable to those obtained from experiments.

TRIO-U (Version V1.4.4)

Non-nuclear specific test cases used as a validation database are listed here.

Laminar flow (for incompressible, Boussinesq and low Mach number regimes)

Basic tests for convection, diffusion and coupled problems:

> 2D Poiseuille flow; 2D axi-Poiseuille; 3D Poiseuille; 2D and 3D Taylor-Green vortices; 2D axi-symmetric pipe flow, with and without conjugate heat transfer; boundary layer on a vertical plate; flow past a 2D circular cylinder (Re=100); oscillating flow in non-symmetrically heated cavity; square box with a moving wall.

Turbulent flow (incompressible, Boussinesq and low mach number regimes)

(a) Mixing length model:

> flow in a turbulent periodic channel; flow in a turbulent periodic pipe.

(b) k-epsilon model:

2D axisymmetric pipe flow, with and without varying sections; 2D Hill flow; heated square box with unsteady thermal stratification with air inlet and outlet; differentially heated square box; S-shaped channel; flow around a single cube and around buildings (from the EEC TRAPPOS project).

(c) LES modelling / RANS-LES hybrid model:

Freely decaying homogeneous isotropic turbulence; isothermal turbulent periodic channel/pipe flow with and without wall functions; differentially heated channel flow with and without wall functions, and with and without solid wall coupling; vertical impinging jet; flow around circular or square cylinders (from ERCOFTAC database); LES on specific nuclear applications.

Porous medium

(a) Air flow through a particle bed; air flow in a storage room with axial arrays of heating tubes; Blasius flow with regular loss of pressure; Blasius flow with mixed open medium and porous medium.

Radiation module

(b) 2D and 3D square cavity with 2 facing walls at imposed temperature and 2 facing perfectly reflecting walls; 2D and 3D axisymmetric cylinders; 2D and 3D square cavity filled with steam (for radiation in absorbing media).

Nuclear specific test cases

Some comparisons between experiments and CFD results have been performed. These include data from the ROCOM 1/5th scale reactor of FZR (Forschungszentrum Rossendorf), from the ISP-43, from tee-junction configurations, from experiments involving temperature transport, and from dilution in complex geometries .

SATURN (Version 1.1)

Listed below are elements of the validation matrices of this EDF in-house code; both nuclear and non-nuclear items are included.

1. Flow around an isolated cylinder: laminar, unsteady, isothermal regime
2. Flow in a 2D square cavity with moving wall: laminar, steady, isothermal regime
3. Taylor vortices: laminar, unsteady, isothermal regime
4. Plane channel flow: laminar and turbulent, steady, isothermal regimes
5. 2D Flow over a hill: turbulent steady, isothermal regime
6. 2D flow in a 2D arrays of tubes: turbulent, steady and unsteady, isothermal regime
7. Flow in a 2D channel with inclined pressure drop: laminar, steady, isothermal regime

8. Freely decaying homogeneous isotropic turbulence: turbulent, unsteady, isothermal regime

9. 3D flow in a cylindrical 180° curved pipe: steady, turbulent, isothermal regime

10. 3D flow around a car shape: steady, turbulent, isothermal regime

11. Natural convection in a 2D closed box with vertical heated walls: steady, turbulent, natural-convection regime

12. Mixed convection in a 2D cavity with air inflow and heating: steady, turbulent, mixed-convection regime.

13. Mixed convection in a 2D cavity with heated floor and air circulation heating: steady, turbulent, mixed-convection regime.

14. 2D axisymmetric jet impingement on a heated wall: steady, turbulent, forced-convection regime.

15. 2D axisymmetric jet of sodium: steady, turbulent regime with thermal transfer

16. Thermal stratification in a hot duct with cold water injection: steady, turbulent, stratified regime

17. Injection (at 45°) of a mixture of gases in a pure gas: steady, turbulent, multi-species flow

18. 2D channel with thick heated walls: steady, turbulent flow with thermal coupling

19. Premixed combustion: steady reactive turbulent flow

20. Diffusion flame: steady, reactive, turbulent flow

21. Pulverised coal furnace: steady, turbulent, reactive flow with radiation heat transfer

22. Two-phase gas/particle flow along a vertical plate: steady, turbulent flow with Lagrangian transport

23. Two-phase gas/particle flow in a vertical cylindrical duct: steady, turbulent flow with Lagrangian transport

24. Industrial tee-junction: steady, turbulent flow

25. Industrial cold water injection in hot water duct: unsteady, turbulent flow with heat transfer

26. Simple tests of functionalities of practical interest (parallelism, periodicity, restart…)

27. Analytical case of radiative transfer in a closed cavity: steady, radiation heat transfer

Cast3M (including TONUS)

Listed below are elements of the validation matrices of two CEA in-house codes; both nuclear and non-nuclear items are included.

Test of scalar equation transport (academic test cases)

a. Convection: 2D rotational transport flow

b. Convection-diffusion: 2D Smith-Hutton flow

c. Non-linear conservation law: 2D Burgers equation

d. Diffusive transport: 2D and 3D heat equation

Radiation heat transfer

a. Transparent media: square cavity, wedge, co-axial cylinders, co-centric spheres, cube

b. Radiation and conduction: air-filled cylinder

c. Absorbing media: absorbing gas in a sphere

d. Radiation and natural convection in absorbing media: 2D square cavity

Single Component Flow

(a) Incompressible

i. Lid-driven cavity

ii. Blasius flat plate

iii. Backward-facing step

(b) Boussinesq

iv. Natural convection in zero Prandtl fluid

v. Rayleigh-Marangoni convection

vi. Vahl Davis differentially heated cavity

(c) Low Mach Number

vii. Differentially heated cavity with large temperature differences

viii. Pressurisation

(d) Compressible Flows

ix. 2D Laval-type nozzles or channel flow; 1D SOD shock tube; 1D double rarefaction wave; shock collisions; moving or steady contact waves; moving or steady shock waves; 1D blast wave; 2D shock reflection; 2D inviscid shear layer; 2D jet interaction; odd-even decoupling; “Carbuncle Test Case”; double Mach reflection; forward-facing step; shock diffraction over 90^{o} corner.

(e) Multi-Component Flows

x. Low Mach and compressible approaches

1. shear layer; non-reactive shock tube; reactive shock tube

(f) Turbulence Modelling

xi. Incompressible k-eps: grid turbulence; fully-developed channel flow; turbulent natural convection in a square cavity

xii. LES on specific experiments

xiii. k-eps and Mixing-Length model for low Mach number NS Equations with condensation

xiv. k-eps for low Mach number reactive flows (EBU modelling)

(g) Containment

xv. MISTRA tests

1. Wall condensation experiment

2. Condensation + convection + conduction in axisymmetric and 3D geometries, with and without He

xvi. Flow in 3D compartmented geometries

xvii. Spray dynamics, with convective heat transfer

xviii. Droplet heat and mass transfer

xix. Spray experiments

xx. H2 detonation in 1D, 2D and 3D geometries

xxi. Fast and slow H2 deflagrations

xxii. LP models with H2 recombiner, with stratification and distribution, with wall condensation

xxiii. Air/steam leaks in idealised and concrete cracks

(h) “GCR” Specific Models

xxiv. Conduction, radiation, convection in complex geometries

xxv. Turbine blade deblading

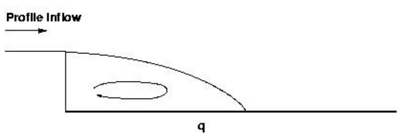
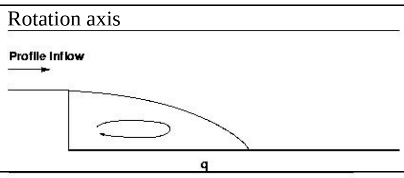
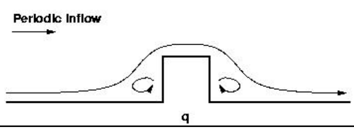
ANSYS (CFX)

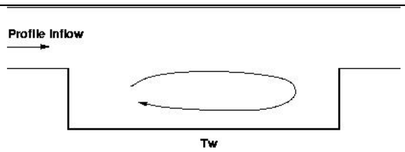
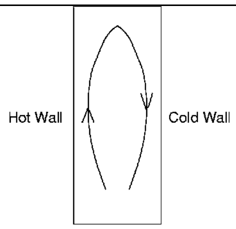
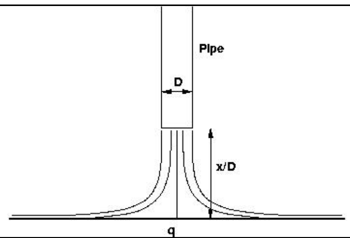
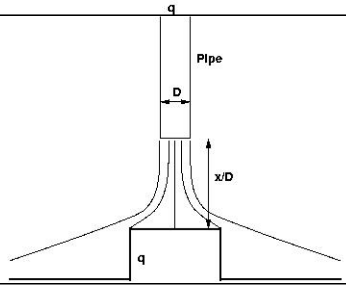
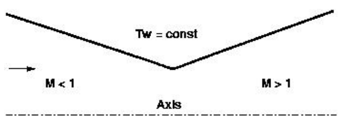
Heat transfer predictions from the two codes CFX-TASCflow and CFX-5 are comprehensively covered in the document cited below. All situations analysed were for turbulent flow conditions. Three two-equation, eddy-viscosity turbulence models were analysed in the context of 9 test cases, illustrated in the accompanying table The test cases are idealised, academic standards, but nonetheless of relevance to NRS issues, since many such situations (though not idealised) will occur in NRS applications. It is estimated that less than 1% of all industrial applications of CFD target the prediction of heat transfer to and from solid walls.

It was found that the often reported poor performance of eddy viscosity models could be attributed to the application of low-Re near wall treatments, and not so much on the underlying turbulence model. It is generally known that k-ε approaches overpredict heat transfer rates in regions of adverse pressure gradient, and at flow-attachment points. The k-ω model has better heat transfer characteristics in near-wall regions, but is sensitive to the free-stream values of ω outside the wall boundary layer. The sensitivity often extends to the specification of inlet values. The SST (Shear-Stress Transport) model is an attempt to take advantage of the favourable characteristics of both models by combining a k-ω treatment near the wall and a k-ε description in the far field. This model performed the best in all 9 test cases, and results compared well with more complex four-equation model v2f, developed at Stanford. On the basis of this benchmark exercise, it was demonstrated that the CFX software is capable of performing heat transfer simulations for industrial flows. The experience gained from this exercise endorses the statement that CFD is a “tried-and-tested” technology, and this has immediate benefits for NRS applications.

Overall, validation is a key component of the CFX software strategy, which is reflected in the vendor’s participation in international benchmarking activities, such as those organised within EU Framework Programmes (ASTAR, ECORA) and ERCOFTAC.

Ref. 1: W. Vieser, T. Esch, F. Menter *“Heat Transfer Predictions using Advanced Two-Equation Turbulence Models”*, CFX Technical Memorandum, CFX-VAL10/0602, AEA Technology, June 2002, florian.menter@ansys.com.

	Experiment	**Mach No & Fluid Properties**	**Flow Type**	**Items of Interest**
Backward Facing Step		Ideal Gas	Plane, 2D	Flow separation, reattachment and re-developing flow, (Vogel & Eaton, 1985)
Pipe Expansion		Ideal Gas	Axi-symmetric	Flow separation, reattachment and re-developing flow, (Baughn *et al.*, 1984)
2D-Rib		Ideal Gas	Plane, 2D	Periodic flow over a surface mounted rib, (Nicklin, 1998)

	Experiment	Mach No & Fluid Properties	Flow Type	Items of Interest
Driven Cavity		Ideal gas	Plane, 2D	Driven cavity flow, (Metzger *et al*., 1989)
Natural Convection		Ideal gas	Plane, 2D	Buoyancy, heat transfer, (Betts & Bokhari, 2000)
Impinging Jet		Ideal gas	Axi-symmetric	Stagnation flow, (Craft et al., 1983,Yan *et al*., 1992)
Impinging Jet on a Pedestal		Ideal Gas	Axi-symmetric	Stagnation flow, (Baughn *et al*., 1993, Mesbah, 1996)
Subsonic and Supersonic Nozzle Flow		0.2 – 2.5, Air-Methane mixture, ideal gas	Axi-symmetric	Cooled turbulent boundary layer under the influence of large pressure gradients, (Back *et al*., 1964)

References

Back, L.H., Massier, P.F. and Gier, H.L., 1964, *"Convective Heat Transfer in a Convergent-Divergent Nozzle"*, Int. J. Heat Mass Transfer, Vol. 7, pp. 549 – 568.

Baughn, J.W., Hoffmann, M.A., Takahashi, R.K. and Launder, B.E., 1984, *"Local Heat Transfer Downstream of an Abrupt Expansion in a Circular Channel With Constant Wall Heat Flux"*, Vol. 106, Journal of Heat Transfer, pp. 789 – 796.

Baughn, J. W., Mesbah, M., and Yan, X., 1993, *"Measurements of local heat transfer for an impinging jet on a cylindrical pedestal"*, ASME HTD-Vol 239, pp. 57-62.

Betts, P. L., and Bokhari, I. H., 2000, *"Experiments on turbulent natural convection in an enclosed tall cavity"*, Int. J. Heat & Fluid Flow, 21, pp. 675-683.

Craft, T. J., Graham, L. J. W., and Launder, B. E., 1993, *"Impinging jet studies for turbulence model assessment – II. An examination of the performance of four turbulence models"*, Int. J. Heat Mass Transfer. 36(10), pp. 2685-2697.

Mesbah, M., 1996, *"An experimental study of local heat transfer to an impinging jet on non-flat surfaces: a cylindrical pedestal and a hemispherically concave surface"*, PhD Thesis, University of California, Davis.

Metzger, D. E., Bunker, R. S., and Chyu, R. K., 1989, *"Cavity Heat Transfer on a Transverse Grooved Wall in a Narrow Channel"*, J. Heat Transfer, 111, pp. 73-79.

Nicklin, G. J. E., 1998, *"Augmented heat transfer in a square channel with asymmetrical turbulence production"*, Final year project report, Dept. of Mech. Eng., UMIST, Manchester.

Vogel, J.C. and Eaton, J.K., 1985, *"Combined Heat Transfer and Fluid Dynamic Measurements Downstream of a Backward-Facing Step"*, Vol. 107, Journal of Heat Transfer, pp. 922 – 929.

Yan, X., Baughn, J. W., and Mesbah, M., 1992, *"The effect of Reynolds number on the heat transfer distribution from a flat plate to an impinging jet"*, ASME HTD-Vol 226, pp. 1-7.

FLUENT

A generally available validation database for Fluent does not currently exist. There are instead three levels of validation reports. The most public are journal publications of validation exercises. Since 1990, more than 100 references have accrued citing validation activities; of these 6 were related to NRS applications. At a second, and more restrictive level, Fluent provides licensed code users (for Universities only the primary holder of the site license) with online access to nineteen validation reports. Titles of the reports are:

- Flow in a Rotating Cavity
- Natural Convection in an Annulus
- Laminar Flow Around a Circular Cylinder
- Flow in a 90 Planar Tee-Junction
- Flows in Driven Cavities
- Periodic Flow in a Wavy Channel
- Heat Transfer in a Pipe Expansion
- Propane Jet in a Coaxial Air Flow
- Non-Premixed Hydrogen/Air Flame
- 300 kW BERL Combustor
- Flow through an Engine Inlet Valve

- Turbulent Flow in a Transition Duct
- Solid Body Rotation with Central Air Injection
- Transonic Flow Over a RAE 2822 Airfoil
- Mid-Span Flow Over a Goldman Stator Blade
- Compressible Turbulent Mixing Layer
- Scramjet Outflow
- Turbulent Bubbly Flows
- Adiabatic Compression and Expansion Inside an Idealised 2D In-Cylinder Engine

The third, and more detailed, set of validation reports exists internal to Fluent. The tests are applied during development of new code versions, but most are proprietary, and details of this validation set are not available externally.

Ref. 1: F. Lin, B. T. Smith, G. E. Hecker, P. N. Hopping, "Innovative 3-D numerical simulation of thermal discharge from browns ferry multiport diffusers", Proc. 2003 International Joint Power Generation Conference, Atlanta, GA, June 16-19 2003, p 101-110.

Ref. 2: R. M. Underhill, S. J. Rees, H. Fowler, "A novel approach to coupling the fluid and structural analysis of a boiler nozzle", Nuclear Energy, 42(2), 95-103 (2003).

Ref. 3: T.-S. Kwon, C.-R. Choi, C.-H. Song, "Three-dimensional analysis of flow characteristics on the reactor vessel downcomer during the late reflood phase of a postulated LBLOCA", Nucl. Eng. Des., 226(3), 255-265 (2003).

6.2 Assessment of CFD codes in their application to NRS issues

ASTAR

ASTAR (Advanced Three-Dimensional Two-Phase Flow Simulation Tool) was a 5th Framework EU shared-cost action dedicated to the further development of high-resolution numerical methods, and their application to transient two-phase flow. The project explored the capabilities of using hyperbolic numerical methods – which are traditionally the province of single-phase fluid dynamics, especially in the aerospace industry – for two-phase flow simulations of relevance to nuclear reactor modelling. Several benchmark exercises were adopted as verification and assessment procedures for comparing the different modelling and numerical approaches.

It was recognised that the simulation tools currently used by the nuclear reactor community are based on elliptic solvers, and suffer from high numerical diffusion. However, many of the accident sequences being modelled with these methods involve propagation of strong parameter gradients: e.g., quench fronts, stratification, phase separation, thermal shocks, critical flow conditions, etc., and such "fronts" become smeared, unless very fine nodalisation is employed. Hyperbolic methods, on the other hand, are well suited to such propagation phenomena, and one the principal goals of the ASTAR project was to demonstrate the flow modelling capabilities and robustness of such techniques in idealised, nuclear accident situations.

ASTAR provide a forum in which separate organisations, developing in-house hyperbolic solvers, could assess their progress within a common framework. To this purpose, a set of benchmark exercises were defined to which the various participants were invited to submit sample solutions. The benchmarks were taken from the nuclear research community, and for which reliable analytical, numerical or experimental data were available. These included: phase separation in a vertical pipe, dispersed two-phase flow in a nozzle, oscillating manometer, the Ransom faucet problem, the CANON (fast depressurisation) test, boiling in a vertical channel, and LINX bubble-plume tests.

Although not all the different numerical approaches (though all hyperbolic) had reached the same level of development and testing, there was evidence coming out of the project that high-resolution, characteristic-based numerical schemes have reached a satisfactory level of maturity, and might therefore be considered as alternatives to the present elliptic-based methods for a new generation of nuclear reactor thermal-hydraulic simulation tool.

Ref. 1: H. Städtke *et al*. "The ASTAR Project – Status and Perspective", 10th Int. Topical Mtg. on Nuclear Reactor Thermal Hydraulics (NURETH-10), Seoul, Korea, Oct. 5-9, 2003.

Ref. 2: H. Paillere *et al*. "Advanced Three-Dimensional Two-Phase Flow Simulation Tools for Application to Reactor Safety (ASTAR)", FISA-2003 / EU Research in Reactor Safety, 10-13 November 2003, EC Luxembourg, http://www.cordis.lu/fp5-euratom/src/ev-fisa2003.htm.

ECORA

The overall objective of the European 5th Framework Programme ECORA is to evaluate the capabilities of CFD software packages in relation to simulating flows in the primary system and containment of nuclear reactors. The interest in the application of CFD methods arises from the importance of three-dimensional effects in these flows, which cannot be predicted by traditional one-dimensional system codes. Perspective areas of the application of detailed three-dimensional CFD calculations is being identified, and recommendations for code improvements are being provided which are necessary for a comprehensive simulations of safety-relevant accident scenarios for future research. Within the ECORA project, the experience of the twelve partners is combined, from European industry and research organisations in the field of nuclear safety, applying the CFD codes CFX, FLUENT, SATURNE, STAR-CD and TRIO_U.

The assessment includes the establishment of Best Practice Guidelines and standards regarding the use of CFD software, and evaluation of results for safety analysis. CFD quality criteria is being standardised prior to the application of different CFD software packages, and results are only accepted if the set quality criteria are satisfied. Thus, a general basis is being formed for assessing merits and weaknesses of particular models and codes on a European-wide basis. CFD simulations achieving the accepted quality level will increase confidence in the application of CFD-tools to nuclear issues.

Furthermore, a comprehensive and systematic software engineering approach for extending and customising CFD codes for nuclear safety analyses has been formulated and applied. The adaptation of CFD software for nuclear reactor flow simulations is being demonstrated by implementing enhanced two-phase flow, turbulence and energy transfer models relevant for pressurised thermal shock (PTS) studies into CFX, Saturne and Trio_U. An analysis of selected experiments from the UPTF and PANDA test series is being performed to validate CFD software in relation to PTS phenomena in the primary system, and severe accident management in the containment.

The selected tests with PTS relevant flow phenomena include free surfaces, stratification, turbulent mixing and jet flows. The test matrix starts with single-effect tests of increasing complexity, and ends with industrially (reactor safety) relevant demonstration cases.

Verification test cases

VER01: Gravitational oscillation of water in U-shaped tube (Ransom, 1992)

VER02: Centralised liquid sloshing in a cylindrical pool (Maschek et al., 1992)

Validation test cases

VAL01: Axisymmetric single-phase air jet in air environment, impinging on a heated flat plate (Baughn and Shimizu, 1989)

VAL02: Water jet in air environment impinging on an inclined flat plate, (Kvicinsky et al., 2002)

VAL03: Jet impingement on a free surface (Bonetto and Lahey, 1993)

VAL04: Contact condensation on stratified steam/water flow (Goldbrunner et al., 1998)

Demonstration test cases

DEM01: UPTF Test 1

DEM02: UPTF TRAM C1

The ECORA web address is http://domino.grs.de/ecora/ecora.nsf. For access to the user forum, contact Martina.Scheuerer@grs.de.

TEMPEST

The shared-cost EU FP5 project TEMPEST focussed on resolving outstanding issues concerning the effect of light gases on the long-term LOCA response of the passive containment cooling systems for the SWR1000 and ESBWR advanced reactors. Validation of multi-dimensional codes for containment analysis was a further objective. A series of five tests in the PANDA facility at PSI, with detailed local measurements of gas species, temperature and pressure, were performed within the project. The experimental data were used for the validation of CFD containment models, and provided improved confidence in the performance of passive heat-removal systems in the presence of hydrogen. CFD codes were successfully employed for predicting stratification behaviour in the containment volumes. This included finding the cause of the tendency of system codes to overpredict containment end-pressure in the presence of light gases. Improved passive containment models for the lumped parameter codes WAVCO and SPECTRA were also validated.

The TEMPEST project was begun to settle the following issues:

1. How does mixing or stratification affect long-term containment pressure response?

2. What are the effects of hydrogen on the performance of passive containment cooling systems?

3. How to apply CFD (and CFD-like) codes for improved passive containment analysis?

A threefold approach was followed. Firstly, PANDA (PSI) and KALI (CEA, Cadarache) experiments were performed in order to provide an experimental database for the above issues. Secondly, CFD models for quantitative assessment of Building Condenser (BC) and Passive Containment Cooling (PCC) system performance were developed and validated. Thirdly, both lumped-parameter and CFD (or CFD-like) codes were then applied to assist in interpreting experimental results, with the objective of better understanding passive containment behaviour.

From the analyses performed within the TEMPEST project, it was found that stratification affects the system end-pressure in these reactors through its effect on the distribution of light gases between the Drywell and the Suppression Chamber. Lumped-parameter codes demonstrated overall satisfactory performance in passive containment analyses, but showed a tendency to overpredict system end-pressure, due to their inability to properly account for stratification. In contrast, CFD codes were shown to be able to accurately predict stratification in gas spaces and water pools, and therefore produce better end-pressure predictions. A combined system-code/CFD-code approach, in which stratification is predicted using CFD, could be considered for future analyses.

Ref. 1: V.A. Wichers *et al*. *"Testing and Enhanced Modelling of Passive Evolutionary Systems Technology for Containment Cooling (TEMPEST)"*, FISA-2003 / EU Research in Reactor Safety, 10-13 November 2003, EC Luxembourg, http://www.cordis.lu/fp5-euratom/src/ev-fisa2003.htm.

IPSS

IPSS is an acronym for European BWR R&D Cluster for Innovative Passive Safety Systems, which was an EU FP4 project concentrating on important innovations of BWRs, such as natural convection in the reactor coolant system and passive decay-heat removal. Experiments were performed at the NOKO (FZJ, separate-effects tests) and PANDA (PSI, integral tests) facilities, and post-test analyses performed with the lumped-parameter/system codes ATHLET, APROS, COCOSYS, MELCOR, RELAP5, TRAC, the containment code GOTHIC, and the CFD codes CFX-4 and PHOENICS.

Though it was demonstrated that traditional lumped-parameter and system codes were capable of reproducing the experimental results, it became evident that CFD codes have to be used to a greater extent than was envisaged at the start of the project. However, it was noted that the validation of these codes for commercial reactor applications was not yet satisfactory, due to the limited amount of relevant experimental data. Nonetheless, the continuing development of CFD codes, and the increasing capacity and speed of computers, the project recognised the usefulness of applying the codes to the analysis of thermal-hydraulic phenomena in real reactors in the future. It was also recommended to continue the study of flow and temperature fields in large water pools and in the containment, and perform further experiments with improved instrumentation (increase in number and sometimes also in quality) in order to accurately resolve regions of stratification, and provide quality data for CFD validation.

Ref. 1: E. F. Hicken, K. Verfondern (eds.) *"Investigation of the Effectiveness of Innovative Passive Safety Systems for Boiling Water Reactors"*, Vol. 11, Energy Technology series of the Research Center Jülich, May 2000.

EUBORA

The EU Concerted Action on Boron Dilution Experiments (EUBORA) had 15 partners, with Fortum, Finland as the coordinator. Most of the partners from the FLOMIX-R project (see below) participated also in EUBORA. The project started in late 1998, and finished within about 15 months.

The primary objective was to discuss and evaluate the needs for a common European experimental and analytical programme to validate the calculation methods for assessing transport and mixing of diluted and boron-free slugs in the primary circuit during relevant reactor transients. The second objective was to discuss how the inhomogeneous boron dilution issues should be addressed within the EU.

The partners concluded that there was a clear need to understand the role of mixing in mitigating the consequences of inhomogeneous boron dilution. In particular, the mixing of a boron-reduced slug on its way from the location of formation to the reactor core inlet is important. In order to take full benefit of this mechanism, one should be able to predict the degree of mixing for the reactor case in the most reliable way. Though 3-D CFD methods do provide an effective tool for mixing calculations, it is important to study the slug transportation in sufficient detail, and to perform the calculations under transient conditions. The code calculations, and the applied turbulent mixing models, have to be validated by experiments. Although a number of small-scale and large-scale tests have been performed in existing facilities, the current status of assessment is deemed to be incomplete. In particular, the large-scale experimental database does not cover all the slug motion and mixing cases.

It was also proposed that cooperation among the existing 1/5-scale experiments would provide useful information by focussing on several phenomenological aspects not yet fully covered by the experimental programmes. It was also concluded that other fluid mixing and flow distribution phenomena should be regarded in the same context, since the final aim is to justify and assess the application of CFD codes for general reactor calculations.

Large-scale experiments (scale 1/2) would provide confirmatory data for the existing 1/5-scale experiments, and the partners supported the proposal to modify the existing PANDA facility at PSI for large-scale mixing experiments, though this has yet to be carried out.

FLOWMIX-R

Fluid mixing and flow distribution in the reactor circuit (FLOWMIX-R) is an EU 5th Framework shared cost action programme with 11 participants, with the Forschnungszentrum Rossendorf, Dresden responsible for project coordination.

1. Forschungszentrum Rossendorf, Dresden (DE)
2. Vattenfall Utveckling AB, Älvkarleby (SE)
3. Serco Assurance, Dorchester, Dorset (GB)
4. GRS, Garching (DE)
5. Fortum Nuclear Services, Vantaa (Fin)
6. PSL, Villingen (SL)
7. VUJE, Trnava (SK)
8. NRI, Rez (CZ)
9. AEKI, Budapest (HU)
10. NPP Paks, Paks (HU)
11. EDO Gidropress, Podolsk (RU)

The project started in October 2001. The first objective of the project is to obtain complementary data on slug mixing, and to understand in sufficient detail how the slug mixes before it enters the reactor core. (Slug mixing is the most mitigative mechanism against serious reactivity accidents in local boron dilution transients.) The second objective is to utilise data from steady-state mixing experiments and plant commissioning test data, to determine the primary circuit flow distribution, and the effect of thermal mixing phenomena in the context of the improvement of normal operation conditions and structural integrity assessment. The third objective is to use the experimental data to contribute to the validation of CFD codes for the analysis of turbulent mixing problems. Benchmark calculations for selected experiments are used to justify the application of turbulent mixing models, to reduce the influence of numerical diffusion, and to decrease grid, time step and user effects in CFD analyses.

Due to the large interest of research organisations and utilities from newly associated states (NASs), a NAS extension of the project, incorporating the research institutions VUJE Trnava, NRI Rez (Czech Republic), AEKI Budapest (Hungary) and the nuclear power plant NPP Paks (Hungary), as well as the research and design organisation EDO Gidropress (Russia), as an external expert organisation, has been undertaken.

The work on the project is performed within five work packages.

In WP 1, the key mixing and flow distribution phenomena relevant for both safety analysis, particularly in steam-line-break and boron-dilution scenarios, and for economical operation and structural integrity, have been identified. Based on this analysis, test matrices for the experiments have been defined, and guidelines have been provided for the documentation of the measurement data, and for performing validation calculations with CFD codes.

In WP 2 on slug mixing tests, experiments on slug mixing at the ROCOM and Vattenfall test facilities have been performed, and the measurement data have been made available to the project partners for CFD code validation purposes. Additional slug-mixing tests at the VVER-1000 facility of EDO Gidropress are also being made available. Two experiments on density-driven mixing (one from ROCOM, one from the Fortum PTS facility) have been selected for benchmarking.

In WP 3 on flow distribution in the cold legs and pressure vessel of the primary circuit, commissioning test measurements performed at the Paks VVER-440 NPP have been used for the estimation of thermal mixing of cooling loop flows in the downcomer and lower plenum of the pressure vessel. A series of quasi-steady-state mixing experiments has been performed at the ROCOM test facility. CFD methods are used for the simulation of the flow field in the primary circuit of an operating full-scale reactor, and computed results compared against available measurement data. Conclusions are being drawn concerning the usability and modelling requirements of CFD methods for these kinds of application.

Concerning WP 4 on validation of CFD codes, the strategy of code validation based on the BPGs, and a matrix of CFD code-validation calculations, has been elaborated. CFD validation calculations on selected benchmark tests are being performed. The CFD validation work is shared among the partners systematically on the basis of a CFD validation matrix.

In WP 5, conclusions on flow distribution and turbulent mixing in NPPs will be drawn, and recommendations on CFD applications will be given.

Quality assurance practice for CFD is being applied, based on the ERCOFTAC BPGs, as specified in the ECORA project for reactor safety analysis applications. Serco Assurance and Vattenfall experts are active in the ERCOFTAC organisation. Most of the FLOMIX-R partners are participating also in ECORA, aimed at an assessment of CFD methods for reactor safety analyses. FLOMIX-R is contributing to the extension of the experimental database on mixing, and the application of CFD methods to mixing problems. Recommendations on the use of CFD codes for turbulent mixing problems defined within FLOMIX-R will be fed back to the ECORA and ERCOFTAC BPGs.

First conclusions from the project are that a new quality of research in flow distribution and turbulent mixing inside the RPV has been achieved in the FLOMIX-R project. Experimental data on slug mixing, with enhanced resolution is space and time, has been gained from various test facilities, and covers different geometrical and flow conditions. The basic understanding of momentum-controlled mixing in highly turbulent flows, and buoyancy-driven mixing in the case of density differences between the mixing fluids, has been improved significantly. A higher level of quality assurance in CFD code validation has been achieved by consistently applying BPGs to the solution procedure.

Ref. 1: F.-P. Weiss *et al., "Fluid Mixing and Flow Distribution in the Reactor Circuit (FLOWMIX-R)"*, Proc. FISA-2003/EU Research in Reactor Safety, 10-13 Nov. 2003, Luxembourg.

ASCHLIM

In the Accelerator Driven System (ADS) concept, thermal neutrons produced by bombarding a high-density target with a proton beam, are utilised to produce energy and for the transmutation of radioactive waste. In some designs, the target material is a Heavy-Liquid-Metal (HLM), which also serves as the primary coolant, taking away the heat associated with the spallation reactions that produce the neutrons. Power densities can easily reach 1000 W/cm^3, not only in the liquid metal, but also in critical structures surrounding the spallation region. Structural materials work at very high temperatures, and have to themselves dissipate large quantities of heat. It is essential to have CFD tools capable of reliably simulating the critical phenomena that occur, since it is not possible to experimentally simulate the acquired power densities without actually using a beam.

The ASCHLIM project (Assessment of Computational Fluid Dynamics Codes for Heavy Liquid Metals) is an Accompanying Measure of the Euratom 5th Framework Programme), and aims at joining different experiences in the field of HLMs, both, in the experimental and numerical fields, and creating an international collaboration to (1) make an assessment of the main technological problems in the fields of turbulence, free surface and bubbly flow, and (2) coordinate future research activities.

Where possible, the assessments have been made on the basis of existing experiments, whose basic physical phenomena are analysed through the execution of calculational benchmarks. Selected commercial codes are used, because of their widespread availability, robustness and flexibility. In some particular cases, research codes belonging to particular research institutes have also been considered, given the fact that they often contain state-of-the-art numerical schemes and models. Particular attention is paid in the project to problems associated with turbulence modelling for HLMs, especially those associated with turbulent heat transfer (i.e. uncertainties in specifying the turbulent Prandtl number), free-surface modelling (in the windowless ADS concept, the beam impinges on the liquid surface) and bubbly flows (one ADS design incorporates gas injection to enhance natural circulation).

Some important indications about the use of CFD turbulence models have come from the ASCHLIM benchmarking activity, although in some cases only partial conclusions could be drawn, principally due to the lack of experimental measurements of turbulence quantities. The most important point to be clarified is the exact range of applicability of the turbulent Prandtl number approach to HLM flows, and possibly to extend it through the formulation, if it exists, of a relationship between it and the local fluid and flow characteristics (e.g. molecular Prandtl number and turbulent Reynolds number), valid at least in the range of Peclet numbers of interest for ADS applications.

Further benchmarking exercises in relation to free-surface configurations, and in particular new experiments with water, are recommended. (The use of water as stimulant fluid arises because the measurement possibilities with water are much broader, and less expensive, than with HLMs.) However, the final assessment clearly must involve experiments with the real, or very similar fluids, (PbBi, Hg).

The need for full 3-D simulations was stressed by most of the participants. However, it must be pointed out here that such simulations could lead to very large, if not prohibitively excessive, CPU times, at least with the present generation of computers. New developments with research codes might also improve the basic knowledge and understanding of free-surface behaviour.

Ref. 1: B. Arien (Ed.) *"Assessment of Computational Fluid Dynamics codes for Heavy Liquid Metals"*, Final Technical Report, October 2003.

Aix-en-Provence May 2002 Exploratory Meeting

The meeting was in two parts: first, several presentations were given describing CFD applications to relevant NRS issues, and then a working group, under the joint chairmanship of J. C. Micaelli (IRSN) and J. Mahaffy (PSU), was convened, with the purpose of defining an action plan on the "application of CFD to nuclear reactor safety problems". This initiative was followed up at the subsequent IAEA/NEA Technical Meeting in Pisa (see below), where further discussions took place, and became the starting point of the present activity.

The technical presentations covered the areas listed here.

- Recent IRSN work on the application of CFD to primary-system-related phenomena (induced breaks, hot-leg temperature heterogeneity and PTS) and containment-related (development and use of the TONUS code) phenomena.

- The ECORA (Evaluation of Computational Methods for Reactor Safety Analysis) 5th Framework Programme.

- The application of in-house codes at NUPEC to provide the Japanese Regulatory Authority with an independent means of assessment of safety analysis of APWR internals. The issues addressed included flow distribution into the neutron reflector (an innovative design improvement), turbulent flow in the downcomer, γ-heating of the neutron reflector, and flow-induced vibrations.

- Mixing of containment gases (relating to ECORA, ISP-42 activities), aerosol deposition (PHEBEN-2 project), wall condensation, liquid-gas interface tracking, and bubble dynamics in suppression pools.

- Application of CFD techniques associated with various EU projects, including PHEBEN-2, TEMPEST, ECORA and NACUSP.

- The need for two-phase CFD in NRS, including details and preliminary conclusions from the EUROFASTNET project, and the latest R&D developments embodied within the joint CEA/EDF code NEPTUNE.

- Some NRS applications requiring CFD: boron dilution, thermal fatigue, induced pipe rupture, PTS, long-term waste storage, together with latest developments of the CEA code TRIO-U.

All the items covered at this meeting have been identified as topics relevant to the activities of this group, and information concerning them is itemised elsewhere in this report. Consequently, no further explanation is given here. A CD-ROM was prepared of the presentations, but no written papers were required.

Ref. 1: *"Exploratory Meeting of Experts to Define an Action Plan on the Application of Computational Fluid Dynamics (CFD) Codes to Nuclear Reactor Safety Problems, Working Group on the Analysis and Management of Accidents"*, Aix-en-Provence, France, 15-16 May, 2002, NEA/SEN/SIN/AMA(2002)16.

IAEA/NEA Technical Meeting, Pisa, November 2002

The meeting was convened to provide an international forum for the presentation and discussion of selected topics related to various applications of CFD to NRS problems, with the intention to use the material presented to identify further needs for investigation. There were 31 oral and 16 poster session presentations, the principal areas covered being PTS, boron dilution, in-vessel mixing, in-vessel severe accidents, containment studies, combustion and two-phase modelling. Presentations and papers are available on CD-ROM.

Ref. 1: *"Technical Meeting on the Use of Computational Fluid Dynamics (CFD) Codes for Safety Analysis of Reactor Systems, including Containment"*, IAEA-OECD/NEA Joint Meeting, Pisa, Italy, 11-14 November, 2002.

OECD/CSNI Workshop in Barcelona 2000

This was the follow-up meeting to that held at Annapolis in 1996, and was intended to review the developments in the areas which had been identified at that time for special focus, to analyse the present status of current thermal-hydraulic and neutronics codes, and to evaluate the role of such tools in the evolving regulatory environment. Though the focus of the meeting, as at Anaheim, remained on system codes, some time was spent on the emerging role of CFD in NRS issues. In the findings and recommendations, it was recognised that CFD involvement was required in areas where the details of local flow behaviour was of importance, and identified thermal stratification and boron dilution as two such areas.

It was recognised (GRS) that though CFD had its roots outside of the nuclear industry, it was attractive to apply a product with proven capability and a large user community in reactor applications. Of particular advantage is the fact that CFD can be readily applied in regions of geometric complexity, and have the capability of modelling turbulence in those situations where it is the dominant flow mechanism, such as for PTS or containment mixing. Everywhere it was emphasised that the major achievements of CFD are for single-phase flows, and that considerable research effort needs to be expended on the physical modelling side if this success is going to be extended to the two-phase flow situations relevant to NRS problems. Some early advances are cited for dispersed flow and the simulation of nucleate boiling using mechanistic models, and a "concerted action" within Germany was announced, involving research centres, university institutes, GRS, a major code vendor and parts of industry, whereby the code CFX-5 would be further developed for the specific needs of the nuclear industry.

Also emphasised at the Workshop was the need to couple CFD modules with system codes, since it was hardly feasible to model all reactor components using a CFD-type discretisation. Generally, it was recognised that for some important transients (boron dilution and PTS) system codes introduced excessive numerical diffusion, due to the use of first-order difference schemes and coarse meshes, that front-tracking methods in these codes did not improve matters, and that CFD was needed to obtain reliable estimates of the degree of flow mixing taking place.

Otherwise, the capabilities of CFD, and its proven worth in non-nuclear applications, was acknowledged, but that considerably more work on two-phase modelling – meaning closure laws and turbulence – was needed.

Ref. 1: Advanced Thermal-Hydraulic and Neutronic Codes: Current and Future Applications, OECD/CSNI Workshop, Barcelona, Spain, 10-13 April, 2000, NEA/CSNI/R(2001)9.

6.3 Proposal for continuation of the assessment matrix and action plan

The present Writing Group has provided evidence to show that CFD is a tried-and-tested technology, and that the main commercial CFD vendors are taking active steps to quality-assure their software products, by testing the codes against standard test data, and through their participation in international benchmark exercises. However, it should always be remembered that the primary driving forces for the technology are non-nuclear: aerospace, automotive, marine, turbo-machinery, chemical and process industries, and to a lesser extent for environmental and biomedical studies. In the power-generation arena, we again find that the principal applications are non-nuclear: combustion dynamics for fossil-fuel burning, gas turbines, vanes for wind turbines, etc. Furthermore, the applications appear to be mainly focussed at design optimisation. This is perhaps not surprising, since CFD can supply detailed information at the local level, building on a design originally conceived using traditional engineering approaches (though themselves computer-aided).

The most fruitful application of CFD in the nuclear power industry seems not to be a support to design, but rather in the Nuclear Reactor Safety (NRS) area. Fitting this application area into the “World of CFD” would appear to represent new challenges to the CFD technology base. The Writing Group has surveyed current activities, and has identified the existing assessment base. Based on this appraisal, and in anticipation that application areas will grow (e.g. thermal fatigue, erosion, corrosion, in connection with maintaining safety standards for ageing plants), it is our opinion that there is a need for a more concerted assessment effort, focussing directly on the application of CFD codes to NRS problems. We propose the following initiatives within the framework of an OECD/NEA/CSNI sponsored action.

- Form a working group to create, maintain and continuously update a web-based assessment database on the application of CFD to NRS issues, and to look for suitable data for use as a benchmarking activity from existing experiments. Suitable candidates for the benchmark should be single-phase, turbulent flow, should include heat-transfer effects, and be of a configuration of relevance to open NRS issues. Possible areas could be: stratified flows, impinging or buoyant jet flows, unsteady turbulent flows as a cause of thermal fatigue, mixing in complex geometries, etc.

- The working group should also evaluate, and stay in touch with, any current experimental programmes, which have the potential for forming the basis of a future benchmark exercise.

- Set up an OECD/NEA International Workshop entitled “The Benchmarking of CFD Codes for Application to Nuclear Reactor Safety”. The Workshop participation would include experimentalists, presenting high quality data for use in CFD benchmarking, and numerical analysts, presenting topical NRS applications using CFD, and code advancements.

- With GAMA/CSNI approval, the working group would be formed early in 2005 and begin organising for the Workshop to take place in mid-2006. Stockholm or Munich have already been suggested as possible venues, with local organisation provided by Vattenfall or GRS Garching, respectively.

7. FINAL SUMMARY

An assessment had been made by this group of the current capabilities of Computational Fluid Dynamics (CFD) codes to perform trustworthy analyses of Nuclear Reactor Safety (NRS) problems. A list of NRS problems for which CFD analysis is required, or is expected to result in positive benefits, has been compiled, and reviewed critically. The list contains safety issues of relevance to core, primary-circuit and containment behaviour under normal and abnormal operating conditions, and during accident sequences.

The list is as comprehensive as the group could assemble given the time and cost constraints upon it, and contains single-phase and two-phase flow examples, though in the latter case the details are deferred to WG3, the group dealing with the *Extension of CFD Codes to Two-Phase Flow Safety Problems*.

Recognising that CFD was already an established technology outside of the nuclear community, the group drew up a list of the existing assessment bases, and discussed their relevance to the application of CFD to NRS issues. It was found that the databases were principally of two types: those concerned with general aspects of trustworthiness of code predictions (ERCOFTAC, QNET-CFD, FLOWNET), and those focussed on particular application areas (MARNET, NPARC, AIAA). It was concluded that application of CFD to NRS problems can benefit indirectly from these databases, and the continuing efforts to extend them, but that a comprehensive NRS-specific database would be a more useful concept. The multiple efforts to improve the quality and trust in the use of CFD for NRS by means of validation exercises, as summarised in a series of NEA/CSNI documents and articles from Jahestagung Kern-technik, point in the right direction, but needed to be brought into a common assessment database.

The group then identified, from a modelling viewpoint, the gaps in the existing assessment databases, and discussed the methodology for establishing assessment matrices specific to NRS needs. From these discussions, proposals were formalised for assembling, maintaining and extending an NRS assessment database. Details of the proposals are given in Section 6.3.

Finally, the scheduling of the tasks to be undertaken by the Writing Group, the lead organisations and estimates of the manpower effort required, were compiled. Details are given in Annex 1.

ANNEX 1
SCHEDULING

The table below is an estimate of organisational responsibility, level of effort, and schedule for the tasks to be carried out by the Writing Group. It is based on the present group structure, and is subject to changes resulting from any new structure of the group, including replacement and/or new participation.

TASK	**Lead**	**Support**	**Person-days**	**Report to Writing Group**
1. Identification of Working Group	OECD/NEA		1 day	Jan. 2005
2. Initial Revision of Existing Document	PSI	All	3 days	Jan. 2005
2.1 Evaluation of Existing Assessment Matrices	NRI	JNES	10 days	March 2005
2.2 Gaps in Assessment Base	NRI	JNES	5 days	March 2005
2.3 Reference List	U.S. NRC	All	20 days	June 2005
2.4 Revised Document	PSI	All	3 days	Sept. 2005
3. Identification of Suitable Benchmarks, following BPGs				
3.1 Core and HXs	Halden	Vattenfall/JNES	10 days	Jan. 2006
3.2 Primary Circuit	GRS	FZR/CEA	10 days	Jan. 2006
3.3 Containment	CEA	GRS/PSI	10 days	Jan. 2006
4. Organisation of Workshop				
4.1 Announcement and Session/Panel Organisation	OECD/NEA	All	5 days	March 2005
4.2 Local Organisation	Vattenfall		10 days	Sept. 2005
4.3 Review of Papers	PSI	All	15 days	March 2006
4.4 Workshop	Vattenfall/GRS	All	10x2 days	June 2006
4.5 Summary of Workshop/Workshop Report (CD)	PSI	All	10x1 days	June 2006
4.6 Additions to Assessment Matrix	NRI	All	7 days	Sept. 2006

<table>
<tr><th>TASK</th><th>Lead</th><th>Support</th><th>Person-days</th><th>Report to Writing Group</th></tr>
<tr><td>5. Web-Site Enhancement</td><td>OECD/NEA</td><td>All</td><td>1 day</td><td>Sept. 2006</td></tr>
<tr><td>6. Evaluation of Workshop</td><td>PSI</td><td>All</td><td>10x1 days</td><td>March 2007</td></tr>
<tr><td>6.1 Core and HXs</td><td>Halden</td><td>Vattenfall/JNES</td><td>1 day</td><td>Dec. 2006</td></tr>
<tr><td>6.2 Primary Circuit</td><td>GRS</td><td>FZR/CEA</td><td>1 day</td><td>Dec. 2006</td></tr>
<tr><td>6.3 Containment</td><td>CEA</td><td>GRS/PSI</td><td>1 day</td><td>Dec. 2006</td></tr>
<tr><td rowspan="2">6.4 Recommendations for the Future</td><td>PSI</td><td>PSU</td><td>2 days</td><td>March 2007</td></tr>
<tr><td colspan="4">Activities would include (1) forming a control group, (2) organisation of a possible benchmark exercise, (3) definition of specific BPGs, (4) web-site maintenance, and (5) organisation of further Workshops.</td></tr>
</table>

ANNEX 2

GLOSSARY

General

ADS	Automatic Depressurisation System (or Accelerator-Driven System)
AIAA	American Institute of Aeronautics and Astronautics
ANS	American Nuclear Society
APRM	Average Power Range Monitor
APWR	Advanced Pressurised Water Reactor
ASCHLIM	Assessment of Computational Fluid Dynamics Codes for Heavy Liquid Metals (EU 5th Framework Accompanying Measure)
ASME	American Society of Mechanical Engineers
ASTAR	Advanced Three-Dimensional Two-Phase Flow Simulation Tool for Application to Reactor Safety (EU 5th Framework Programme)
BDBA	Beyond Design-Basis Accident
BPGs	Best Practice Guidelines
CFD	Computational Fluid Dynamics
CMT	Core Make-up Tank
CPU	Central Processing Unit
CSNI	Committee on the Safety of Nuclear Installations
DBA	Design-Basis Accident
DES	Detached Eddy Simulation
DHX	Dumped Heat Exchanger
DNB	Departure from Nucleate Boiling
DNS	Direct Numerical Simulation

DRACS	Direct Reactor Auxiliary Cooling System
DVI	Direct Vessel Injection
ECCOMAS	European Community on Computational Methods in Applied Sciences
ECCS	Emergency Core-Cooling System
ECORA	Evaluation of Computational Fluid Dynamic Methods for Reactor Safety Analysis (EU 5th Framework Programme)
EOC	End-Of-Cycle
ERCOFTAC	European Research Community on Flow, Turbulence and Combustion
EUBORA	Boron Dilution Experiments (EU 4th Framework Concerted Action)
FISA-2003	The Fifth International Symposium on EU Research and Reactor Safety
FLOWMIX-R	Fluid Mixing and Flow Distribution in the Reactor Circuit (EU 5th Framework Shared-Cost Action)
GAMA	Working Group on the Analysis and Management of Accidents
HDC	Hydrogen Distribution and Combustion
HTC	Heat Transfer Coefficient
HPI	High Pressure Injection
HYCOM	Integral Large Scale Experiments on Hydrogen Combustion for Severe Accident Code Validation (EU 5th Framework Project)
IAEA	International Atomic Energy Agency
ICAS	International Comparative Assessment Study
IPSS	Innovative Passive Safety Systems (EU 4th Framework Programme)
IRWST	In-Containment Refuelling Water Storage Tank
ISP	International Standard Problem
JNC	Japanese Nuclear Corporation
JSME	Japanese Society of Mechanical Engineers
LANL	Los Alamos National Laboratory
LBLOCA	Large-Break Loss Of Coolant Accident
LES	Large Eddy Simulation

LFWH	Loss of Feedwater Heating
LOCA	Loss Of Coolant Accident
LPIS	Low Pressure Injection System
LPRM	Local Power Range Monitor
LS	Level Set
MCPR	Minimum Critical Power Ratio
NEA	Nuclear Energy Agency
NRS	Nuclear Reactor Safety
OECD	Organisation for Economic Cooperation and Development
PAHR	Post Accident Heat Removal
PRHR	Passive Residual Heat Removal
PIRT	Phenomena Identification Ranking Table
PTS	Pressurised Thermal Shock
RANS	Reynolds-Averaged Navier-Stokes
RPT	Recirculation Pump Trip
RPV	Reactor Pressure Vessel
RSM	Reynolds-Stress Model
SARA	Severe Accident Recriticality Analysis
SG	Steam Generator
SLB	Steam-Line Break
SM	Structure Mechanics
TEMPEST	Testing and Enhanced Modelling of Passive Evolutionary Systems Technology for containment cooling (EU 5th Framework Programme)
V&V	Verification and Validation
VOF	Volume-Of-Fluid
VTT	Technical Research Centre of Finland

Codes

ABAQUS	Commercial structural analysis program
AQUA	In-house CFD code developed by JNC
ANSYS	Commercial structural analysis program
APROS	In-house thermal-hydraulic code, developed Technical Research Centre of Finland
ASTEC	Accident Source Term Evaluation Code, developed jointly by IPSN and GRS for analysis of severe accidents
ATHLET	System analysis code, used extensively in Germany
CAST3M	General-purpose finite element code, developed by CEA
CATHARE	System analysis code, used extensively in France
CFX	Commercial CFD software program
COCOSYS	Containment code, developed by GRS for severe accident analysis
CONTAIN	Lumped-parameter code, sponsored by the US NRC, for severe accident analysis
DINUS-3	Direct Numerical Simulation (DNS) tool, developed by JNC
FELIOUS	Structural analysis code, developed by NUPEC
FLICA4	3-D, two-phase thermal-hydraulic code, developed by CEA/IPSN
FLUBOX	In-house, two-phase flow code, developed by GRS
FLUENT	Commercial CFD software program
GASFLOW	In-house CFD code developed by FZK
GENFLO	In-house CFD code, developed by VTT
GOTHIC	General-purpose containment code with 3-D capability, developed by Numerical Application Incorporated (NAI)
MCNP	Monte-Carlo Neutronics Program
MELCOR	Lumped-parameter code for analysing severe accidents, developed at Sandia NL
MpCCI	Mesh-based parallel Code Coupling Interface, distributed by STAR-CD/Adapco, used to couple CFD and SM codes
Permas	Commercial finite-element SM program
PHEONICS	Commercial CFD software program

RECRIT	Computer code for BWR recriticality and reflooding analyses, developed by VTT
RELAP5	System analysis code, used extensively in US and elsewhere
SAS4A	Sub-channel code, developed by ANL, used for analysis of severe accidents in liquid-metal-cooled reactors
SATURNE	3D CFD code, developed by EDF
SCDAP	Severe Core Damage Analysis Package, developed at Idaho National Laboratory
STAR-CD	Commercial CFD software program
TONUS	Containment code, developed by CEA under sponsorship of IRSN
TRAC	Transient Reactor Analysis Code
TRACE	TRAC/RELAP Combined Computational Engine
TRIO-U	CFD software program, developed by CEA
VSOP	Code for reactor physics and fuel cycle simulation, developed at FZJ

Experiments

MICOCO	Mixed Convection and Condensation benchmark exercise, based on MISTRA data
MISTRA	Experimental facility operated by CEA Saclay, used for containment studies
MSRE	Molten Salt Reactor Experiment, operated by ORNL
NOKO	Experimental facility at FZJ, used for studies of BWR condensers
PANDA	Integral test facility at PSI for analysis containment transients
PHEBUS	Experimental facility at CEA Cadarache, used for severe accident research
ROCOM	Experimental facility at FZR, used to investigate upper plenum mixing
RUT	Large-scale combustion experimental facility at the Kurchatov Institute, Russia
SETH	Series of experiments, sponsored by OECD, to be performed in the PANDA facility at PSI
UPTF	Upper Plenum Test Facility at FZR, examining LOCA-related phenomena

Reactors

ABWR	Advanced Boiling Water Reactor
ADS	Accelerator-Driven System

BWR	Boiling Water Reactor
EPR	European Pressurised-Water Reactor
ESBWR	European Simplified Boiling Water Reactor
GCR	Gas-Cooled Reactor
GFR	Gas-Cooled Fast Reactor
HDR	*Heissdampfreaktor;* reactor concept using super-heated steam for cooling, now used for containment experiments, situated at Karlstein, Germany
HTGR	High Temperature Gas-Cooled Reactor
HTR	High Temperature Reactor
KONVOI	Siemens-KWU design of EPR
LMFBR	Liquid Metal Fast Breeder Reactor
LWR	Light Water Reactor
NPP	Nuclear Power Plant
PWR	Pressurised Water Reactor
SWR-1000	*Siedenwasserreaktor* (Boiling Water Reactor)-1000
VVER	Russian version of the PWR