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VALIDATION AND VERIFICATION OF FLOWNEX NUCLEAR

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ABSTRACT

This paper provides a summary of the Software Verification and Validation (V&V), which has been performed on the nuclear safety-relevant elements in Flownex that are currently used in the Pebble Bed Modular Reactor (PBMR) safety case. M-Tech Industrial (M-Tech) and PBMR have embarked on a rigorous V&V process to guarantee the integrity of engineering analyses and to satisfy the statutory requirements regarding the licensing and operating of nuclear plants in South Africa and abroad.

Tools used in the verification of Flownex Nuclear include test plans and procedures, code reviews, user testing, automated testing and regression testing; all implemented under an ISO 9001:2000 quality management system at M-Tech, the code developers. Validation of Flownex Nuclear is performed by comparing the results of the theoretical models with benchmark data obtained from appropriate methods or sources such as analytical data, experimental data, plant data and data obtained form other codes such as Spectra, XNet and Star CD in both separate effect and integrated tests. To further enhance the Flownex V&V effort and to ensure that the Flownex capabilities comply with the latest requirements on High Temperature Gas Reactor (HTGR) analysis, M-Tech is an active participant in international standard problems and conferences, like CRP-5, ICAPP and HTR-TN.

INTRODUCTION

The Flownex Nuclear software started in 1986 with the development of a code based on the Hardy-Cross method to solve air distribution networks for aero belt conveyer systems called Flownet. In 1988 Flownet was extended to deal with complete aircraft air conditioning systems and fuel systems. The Implicit Pressure Correction Method (IPCM) [1] solution algorithm was developed in 1990. In 1992 Rolls-Royce started to use Flownet to simulate aircraft combustion systems. In 1997 the code obtains the capability to analyse transient flows and in 1999 Flownet 4.9 was extended to simulate the PBMR. During 2000 gas mixtures and conduction heat transfer elements where added to Flownet 5.2.

During 1999 M-Tech was contracted by PBMR to redevelop Flownet within a strict ISO 9001 quality framework. The program was to be written in C++ in an object-oriented paradigm and a relational database would be used to store the network data and characteristics such as fan and pump curves, turbine and compressor maps.

In 2001 the code's name was changed to Flownex due to the Flownet name already being registered internationally. Later that same year Flownex Nuclear 6.0 was released.

Flownex Nuclear is thus being developed to perform thermal-hydraulic analyses on a high temperature gas cooled reactor as part of a direct, recuperated Brayton cycle in an implicit way. Various verification and validation methods from diverse sources are used to qualify the software. The fact that Flownex Nuclear is the first software product to be developed for the integrated thermal hydraulic analysis of the complete HTR Brayton cycle should be stressed as it impacts on the availability of independent software products and experiments that can be used for software V&V activities.

PBMR uses Flownex Nuclear to calculate mass flows, temperatures and pressures in the reactor core and the Brayton cycle during expected operational modes and states and under accident conditions. Flownex Nuclear is used for both steady-state and transient simulations.

Simulation results are fed back into the design process, where it dictates plant layout, material selection and operating philosophies. The accuracy of these simulations is crucial in determining the safety of operation, economic viability and protection of the plant.

M-Tech and PBMR have embarked on a rigorous V&V process to guarantee the integrity of engineering analyses and to satisfy statutory requirements regarding the licensing and operating of nuclear plants in South Africa and abroad. Verification and validation of individual components as well as integrated systems of components for both steady-state and transient analysis is required. To date approximately 70 000 man hours have gone into this V&V effort.

NOMENCLATURE

CRP-5	: Coordinated research project
EES	: Engineering Equation Solver
HPTU	: High Pressure Test Unit
HTGR	: High Temperature Gas Reactor
HTF	: Helium Test Facility
HTR-TN	: High Temperature Reactor Technology Network
HTTF	: Heat Transfer Test Facility
HTTU	: High Temperature Test Unit
ICAPP	: International Congress on Advances in Nuclear Power Plants
IPCM	: Implicit Pressure Correction Method
NNR	: National Nuclear Regulator
V&V	: Verification and Validation
PBMR	: Pebble Bed Modular Reactor
SANA	: Self acting removal of after heat
Spectra	: Sophisticated Plant Evaluation Code for Thermal-hydraulic Response Assessment
XNet	: Explicit thermal-fluid network code

THE V&V PROCESS

The V&V process for a component in Flownex starts with the creation of a theory manual. These theory manuals describe the theoretical derivation of equations used in the particular Flownex component and justify any simplifying assumptions made in their derivation. Theory manuals also provide details on fundamental mass, momentum and energy conservation as applied to each Flownex component or feature. Currently there are 33 Flownex theory manuals which total 800 pages.

Flownex validation manuals are then created to provide comparisons with benchmark data for the various validation cases as defined in the phenomena charts. To date, 50 validation manuals have been written totaling more than 2000 pages. In the comparison of Flownex with benchmark data, acceptance criteria were established to aid in the determination of successful verification or validation. These acceptance criteria will be discussed later in section 2.5.

In order to ensure that the software V&V has been performed on an acceptable standard and that all various aspects of the software V&V process have been thoroughly addressed per element, a V&V review and technical closeout meeting is held by M-Tech and PBMR specialists. During these meetings, the whole software V&V programme for the element is discussed and evaluated to ensure that the software V&V complies with technical and regulatory requirements.

M-Tech compiled a Final Software V&V Report to conclude the V&V effort for the nuclear safety components, summarising the software V&V activities, tasks and results. The overall software quality is also assessed in the Final software V&V Report.

V&V ACTIVITIES

In order to ensure that all phenomena for each component in Flownex Nuclear are validated for the various extremities, validation cases were selected to cover the full range of thermal-hydraulic phenomena listed in the Flownex Nuclear Phenomena Charts.

The Flownex software V&V effort is applicable to the complete Flownex software product with priority given to the elements that are used in nuclear safety-relevant calculations.

BENCHMARK AND EXPERIMENTAL COMPARISONS

The validation cases consist of a mix of analytical solutions, experimental data, and other calculation methods.

Various experimental facilities are used to aid in the software V&V effort:

Smaller thermal-hydraulic facilities at North-West University are used to validate phenomena on the pipe, node, heat exchanger and valve components in Flownex. These experiments are:

FXEX001-VOL: Transient volume blow down experiment.
FXEX001-HEX: Transient heat exchanger experiment.
FXEX001-TRA: Fast transient pipe network experiment.
FXEX001-NET: Steady-state complex pipe network experiment.
FXEX002: Shell & Tube heat exchanger steady-state and transient experiment.

Data from these facilities have been incorporated into the validation activities.

The Pebble Bed Micro Model (PBMM) at North-West University is used to gather data for separate and integrated effects validation of Flownex. This data is used for the validation of both steady-state and transient phenomena.

The Heat Transfer Test Facility (HTTF) at North-West University will be used to compare heat transfer and flow phenomena in the reactor model in Flownex with experimental results. The HTTF consists of two facilities, the High Pressure Test Unit (HPTU) and the High Temperature Test Unit (HTTU) which will be finished September 2006 and mid 2007 respectively.

Experiments performed at the SANA experimental facility in Germany have been used in the software V&V of heat transfer phenomena in the reactor model in Flownex.

The Helium Test Facility (HTF) in Pelindaba will be used to compare several flow, pressure and temperature related phenomena of Helium and PBMR related components with Flownex models.

Alternative steady-state and transient calculations on the Flownex software models and on integrated calculation models are performed with the independently developed software code XNet.

XNet is a general thermal-hydraulic network code, capable of solving complex thermal-hydraulic networks. Whilst Flownex is based on a wide range of element types from very simple to very complex models, XNet is based entirely on primitive elements. These elements are the fundamental elements necessary for modeling any thermal-hydraulic problem. Each primitive element addresses only a single phenomenon, whilst a Flownex element may address several phenomena simultaneously. XNet uses an explicit fourth order Runge-Kutta time integration scheme with trapezoidal damping to solve the one-dimensional governing equations, as opposed to the implicit pressure correction method (IPCM) employed by Flownex. This implies that

XNet solves primary variables that are different from Flownex.

Alternative steady-state and transient calculations on component models and on the integrated PBMR MPS calculation model have also been performed by the Nuclear Research and consultancy Group (NRG), using their SPECTRA software code.

Software sensitivity studies are performed as part of the Flownex Nuclear software V&V. Boundary conditions, material properties and physical models, (e.g. the inlet area, or loss coefficients) are varied systematically within accuracy limits. The results are then compared with benchmark solutions to establish if any cliff edge effects occur due to the solution algorithms or other software related sources.

Before any steady-state Flownex result can be compared to a benchmark, a grid independent solution must be obtained. This is done by raising the number of increments until there is only an insignificant change in the results. Grid independence is especially important when non-linear problems are simulated such as choking in a pipe due to the linear simulation approach Flownex uses. In the event of a transient validation case time-step independence must also be insured. These results can then be compared with the benchmark solutions.

COMPARISONS WITH ANALYTICAL SOLUTIONS

Most of the analytical solutions used in the V&V effort have been obtained using EES (Engineering Equation Solver). EES is a commercial off-the-shelf product with the basic function to provide numerical solution of a set of algebraic equations. It can also solve differential and integral equations, do optimization, provide uncertainty analyses, and perform linear and non-linear regression.

COMPARISONS WITH ALTERNATIVE MODELS AND PEER REVIEW

To enhance the Flownex software V&V effort and to ensure that the Flownex capabilities comply with the latest requirements on HTGR analysis, M-Tech is an active participant in international standard problems and conferences. M-Tech has participated in the Fifth Research Coordination Meeting (RCM) for CRP-5 on HTGR Performance Evaluation which was held in, Vienna - Austria in 2004 and is currently solving the benchmark problem as proposed during the Sixth RCM for CRP-5 on HTGR core physics & thermal-hydraulic code benchmarks, the introductory meeting of which was held in September 2005, also in Vienna. M-Tech is currently working to complete sections of the Techdoc II of CRP-5 for the seventh RCM to be held in Vienna in September 2006.

Various conference articles were also published and presented at the HTR-2004 Conference on High-Temperature Reactors in Beijing, China and at the HTR-2002 Conference on High-Temperature Reactors in Petten, the Netherlands.

As soon as milestones in the development and V&V of Flownex were reached, presentations were given to the Flownex users at PBMR. These presentations would generally result in critical questions by the experienced users, providing worthwhile feedback for the Flownex V&V effort as well as giving all users a better comprehension of the Flownex software.

V&V OF THE SOLVERS

Three different solvers are implemented in Flownex, a pressure, temperature and concentration solver. Flownex also employs a state-of-the-art implicit pressure correction solution algorithm that results in fast and accurate simulations. The various steps involved in the implicit pressure correction algorithm are listed in the Flownex user manual and Flownex IPCM theory manual. In these steps continuity is checked. Flownex can only give results if there is conservation of all conservation equations three (mass, momentum and energy).

In order to verify the different solvers according to the NNR requirements three validation manuals were created, one for each solver, this focused on the conservation of the three conservation equations. In fact, in all the V&V cases the results as given by the solvers are compared to benchmarks and thus are the solvers also verified.

ACCEPTANCE CRITERIA FOR COMPONENT VALIDATION

The following literature survey was conducted to establish a baseline for the acceptance criteria:

VALIDATION METRICS

The specification and use of validation metrics is one of the most important practices in validation activities. Oberkampf et al. [1] stated that one of the four factors necessary for a strong benchmark is an exact, standardized, frozen and promulgated definition of acceptance criteria for comparison of codes with the benchmark's results. These acceptance criteria or validation metrics are used to quantitatively compare the results of code calculations with the results of validation experiments. The word ”metrics” is simply interpreted as “measures”. Thus, the choice of one or more metrics defines the means used to measure the differences between computational results and experimental data [1].

These metrics include uncertainties and errors as presented in [9] and which can be sub-divided in:
Numerical errors: Solution or discretization errors, iteration errors, round-off errors.
Model errors: Inadequacies of selected models.
User errors: Lack of expertise in geometry and grid generation, definition of boundary conditions, selection of solver parameters, post-processing.
Application uncertainties: Lack of information on geometry and boundary conditions (turbulence quantities, inlet profile shapes).

Considering these uncertainties and errors any comparison for model validation naturally leads to the following questions:

When is the agreement between benchmark data and the model predictions sufficient, and how should this agreement be quantified?

Literature research has shown that acceptance criteria are widely used in V&V activities, but are seldom quantified. Target variables are usually defined, but only a few researchers have defined quantitative acceptance criteria.

LITERATURE EXAMPLES

An example of criteria used to establish the adequacy of the scientific basis for the comparisons of thermal transport model output (velocity and temperature distribution) with experimental data are 25 percent and 5 percent for comparisons with analytical and numerical solutions [3]. Heiring et al. [4], stated that eight participants calculated the thermal-hydraulic conditions, for the Quench-06 experiment (flooding of the overheated reactor core with water as part of an accident management measure), fairly well and delivered results in the range of ± 15 percent around the experimental value. Wolters et al. [5] described that, with respect to calculated temperatures, the results of single codes and turbulence models lie within a margin of about 15 percent and therefore agree quite well.

In a Relap5/Mod3 [6] reflooding validation case, the researchers stated that a stand-alone validation of the new model has shown acceptable agreement with the data with a standard deviation of about 40 percent for the simulation of heat flux. Doval [7] concluded in his validation that a good number of cases have been simulated using the thermo hydraulic package of the MTR_PC v2.6 and results (pressure drop, heat flux and velocity) have been compared against commercial and customized programs results, theoretical values and experimental data. Almost in every case, percentage deviations are within 10 percent and he concluded that the package MTR_PC v2.6 is an appropriate tool to be used for thermal-hydraulic design purposes of research reactor cores. In validating the integral code ASTEC (Evita), Allelein et al. [8] prepared a classification scale to describe the differences in the results between computer platforms: negligible below 0.01 percent, small below 1 percent and acceptable up to 10 percent.

QUANTIFY ACCEPTANCE CRITERIA

It is clear from the above mentioned examples that the acceptance criteria for defined target variables are quantified by the researcher's judgment and experiences and based upon the phenomena being tested. Oberkampf and Trucano [10] state that if the difference between the experimental measurement and the computational result is less than the validation metric (acceptance criteria), then the result is judged validated. M-Tech has defined generic quantitative acceptance criteria for defined target variables in order to have a first cut-off point for the V&V engineer to select cases where further investigation in the differences is required based on the phenomena under investigation. These generic acceptance criteria are stricter than the examples found in literature to ensure acceptability of all validation cases and are based on engineering judgement. They are only applicable to the Flownex Software V&V, which tests the applicability of the software to phenomena that will form part of nuclear safety relevant applications at PBMR. Calculation Model V&V that is to be performed by the PBMR analysts shall have its own applicable acceptance criteria.

It was opted to compare the differences between the benchmark results and the Flownex results using the normalized point difference and the Euclidian difference.

The normalized point difference gives the difference between Flownex and the benchmark for each point divided by the total range of the variable for the system under investigation. This is similar to the "percentage of full scale" used in the specification of the accuracy of instruments. The benchmark data could be measured (experiment or plant data), calculated (analytical) or modeled (other software codes). The following equation is used to calculate the normalized point difference for variable y:

$$e_{NPD} = \frac{\left| y_{FNX} - y_{BM} \right|}{\Delta y_{SYS}} \qquad (2.1)$$

where

y_{FNX} = the Flownex variable,

y_{BM} = the benchmark variable,

Δy_{SYS} = the total range of the variable for the system under investigation.

The Euclidian difference gives the fractional difference between the Flownex results and the benchmark data over the whole range of data points. The following equation is used to calculate the Euclidian difference:

$$e_{Euclidian} = \sqrt{\frac{\sum \left(y_{FNX} - y_{BM} \right)^2}{\sum \left(y_{BM} \right)^2}} \qquad (2.2)$$

The values used are as follows:

For analytical and numerical comparisons, the normalized point difference must be smaller than 1 percent. This allows for round-off errors, differences between numerical methods, computer inaccuracy, etc.

For comparisons with other codes, the Euclidian difference must be smaller than 5 percent. Other codes use different solution techniques and different models, independently developed by different people using different assumptions and therefore a 5 percent Euclidian difference in the results is considered appropriately small.

For comparisons with experimental or plant data the Euclidian difference must be smaller than 10 percent. Due to measurement uncertainties in the experimental data, a 10 percent Euclidian difference between experimental results and the simulation is considered within limits.

Benchmark results that fall within this guideline on the first comparison are deemed acceptable. Should comparisons fall outside this guideline they are investigated further and may still be deemed acceptable. This would need to be justified, however. Equally, if a result would be within the acceptance criteria, but obviously is out of touch compared to similar results, further investigation would be required. It is the responsibility of the V&V engineer to highlight the applicable difference, bring it into context and justify the difference or investigate its cause.

TYPICAL V&V EXAMPLES

In this section a few typical V&V cases will be discussed showing the application of the acceptance criteria. To date, approximately 400 V&V cases have been created.

PIPE ELEMENT

In one of the cases of the pipe V&V effort, the Flownex pipe element is verified for buoyancy flow. A typical U-tube setup is simulated as shown below in Figure 1. The mass flow rate, density, outlet temperature and velocity of Flownex are compared to the analytical benchmark, EES. The maximum normalised point difference for the comparison is negligible at 0.02 percent.

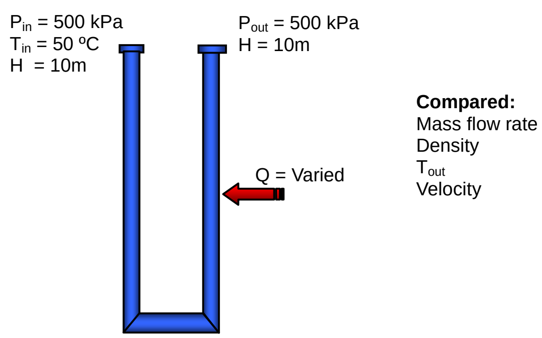

Figure 1: Graphical presentation of Case 8 of the pipe V&V effort.

ADVANCED PEBBLE BED REACTOR MODEL

Case 2 of the advanced pebble bed reactor model is a comparison of a fluid Temperature transient with compressible flow through a pebble bed zone. The fluid temperature and solid temperature throughout the pebble zone is shown in Figure 2, below. The maximum Euclidian difference between Flownex and XNet is 2.05 percent, which can be observed to be negligible in this case.

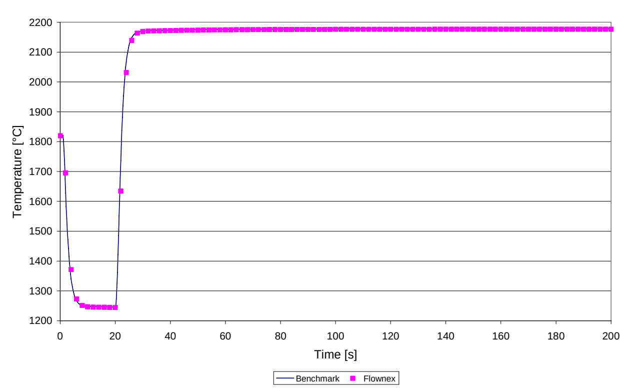

Figure 2: Gas temperature graph of case 2 of the advanced pebble bed component.

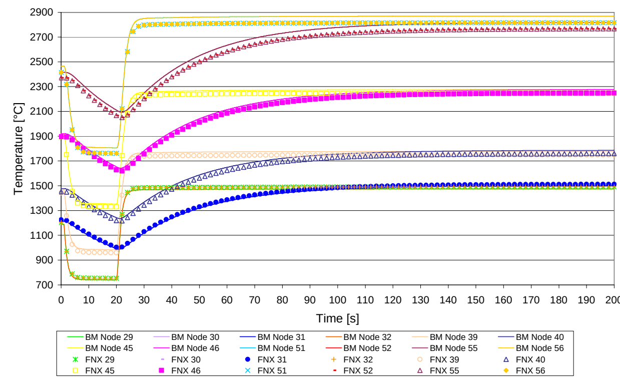

Figure 3: Solid temperature graph of case 2 of the advanced pebble bed component.

NETWORK BALANCING EXPERIMENT

One of the experiments used in the V&V effort is a network balancing experiment, were a complex interconnected pipe network experiment was performed. Ten different steady state experiments were performed. For the first experiment the maximum normalized difference was 7.65 percent and the maximum Euclidian difference was 2.08 percent. It can be observed that the confirmation is remarkable.

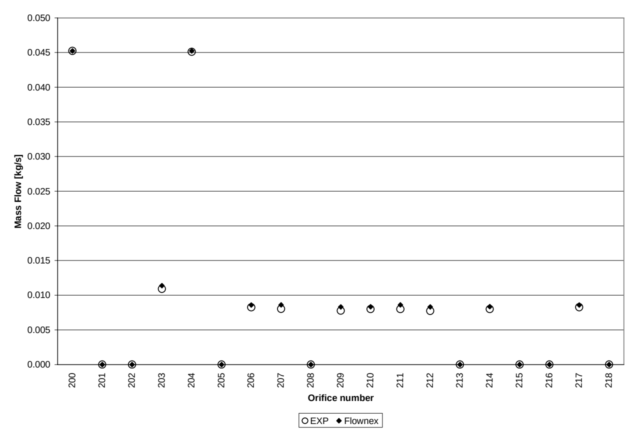

Figure 4: Compared mass flow rates for the network balancing experiment.

VOLUME BLOWDOWN EXPERIMENT

Another experiment used in the Flownex software V&V effort is a volume blow down experiment of three connected tanks. The first tank is filled with 900 kPa (g) of CO_2, the second tank is as at vacuum and the third is filled with air to 450 kPa bar (g). The valves that connect the tanks are simultaneously opened and the blow down graph is shown below. The maximum Euclidian difference for this experiment is 2.94 percent, which is very close as well.

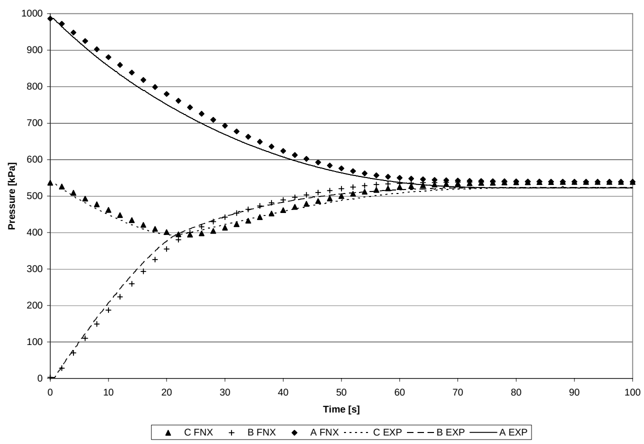

Figure 5: Pressure comparison for the volume blowdown experiment.

CONCLUSION

This paper described the Flownex Nuclear Software V&V effort and process that was followed to V&V the solvers and nuclear safety relevant elements used by PBMR. In this V&V effort Flownex was compared to analytical and numerical benchmarks, other codes, experimental data and plant data. The acceptance criteria that was used in the V&V was thoroughly discussed and several examples shown to illustrate its use. The V&V is judged to be sufficient, within acceptance criteria and a good representation of the phenomena that are simulated. Later versions of Flownex will also be checked against all the V&V networks from the various V&V cases to ensure that future Flownex releases also adhere to the set requirements. M-Tech's continuous international participation in the IAEA Coordinated Research Project (CRP-5) provides Flownex with even more exposure to peer reviews on various platforms.

It can be concluded that Flownex is suitable for use in nuclear safety relevant calculations and simulations of HTGR technology.

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