ANSWERS computer codes: verification and validation for novel reactor applications

ANSWERS codes are used to model general radiation transport. **John Lillington**, **Glynn Hosking**, **Paul Smith** and **Peter Smith** explain the applications of the codes and how they can be used to predict confidently how a wide variety of reactor systems will perform.

There is a need for the continuing development of reactor codes to support novel reactor applications and new advanced reactor designs. The first objective of this paper is to describe and demonstrate the flexibility of the ANSWERS computer codes as tools for modelling the reactor physics and fuel performance of the wide range of different reactor systems under consideration for the future. The second objective is to demonstrate something of the extensive verification and validation (V&V) against research and other reactor data that has underpinned the development of the ANSWERS codes suite in order to provide confidence in predictions.

The ANSWERS codes model general radiation transport, including reactor physics, criticality and shielding. The codes have evolved over 50 years [1] and have been applied to all scales of reactor – from small, zero-power experimental reactors up to large-scale commercial reactors. They have been applied to a very wide range of reactor types, including light and heavy water, gas-cooled and liquid-metal-cooled, thermal and fast systems.

Novel and advanced reactors

Most of the novel and generation IV (Gen IV) advanced reactor concepts are evolutions of current generation reactors or reactors that have operated previously, many for extended periods. These include: small, medium and large-scale water-, gas- and liquid-metal-cooled fast reactors. In some areas, much of the V&V of the codes carried out for these older reactors remains valid for the new proposed reactors, including Gen IV reactors. This is true, for example, for much of the reactor physics and fuel performance modelling in these codes.

There are small modular reactors (SMRs) proposed for relatively near-term deployment that are based on small integral pressurised water reactors (PWRs). Since much of the V&V of the computer codes was carried out through benchmarks and experiments for small and prototype reactors, the codes' V&V is particularly relevant for SMRs and indeed for other small reactor concepts, e.g. fast reactors for plutonium disposition.

ANSWERS software

The ANSWERS codes and consultancy service support reactor operations and nuclear facility-related activities to clients worldwide. These include clients from UK, Europe, North America, Asia (China, Japan and South Korea) and the Middle East (UAE). The modelling services cover: reactor physics, criticality, radiation shielding, dosimetry, nuclear data, fuel performance, thermal hydraulics and structural mechanics (Table 1). Activities cover reactor design and operations, early and late stages of the fuel cycle, waste management, transport flasks design and repository planning assessments.

Light-water reactors

Technology

Current interest is centred on the Gen III and III+ reactor technologies for optimised current generation and near-term new build, and also on the SMRs (small integral PWRs) that might be

Table 1

ANSWERS radiation transport codes

Software	Modelling features
WIMS	Modular reactor physics; pin-cell to whole core geometries
PANTHER	Neutron diffusion and thermal hydraulics, transient analysis
MONK	Nuclear criticality safety; Monte Carlo, advanced geometry
CRITEX	Nuclear criticality excursion analysis in fissile solutions
MCBEND	Radiation shielding and dosimetry; Monte Carlo, advanced geometry
RANKERN	Radiation shielding and dosimetry; point kernel, flexible geometry
TRAFIC	Mechanistic fuel performance; fast reactor oxide, nitride and carbide fuel

deployable in the next 10 years. There is currently little interest in developing advanced Gen IV super-critical water reactors.

R&D requirements

To support these technologies requires the development of new capabilities in the areas of fuels for higher burn-up and extended fuel cycle, reactor physics, thermal hydraulics, chemistry, structural materials and reactor engineering and safety. A priority activity in the longer term is the development of accident-tolerant fuels (ATFs) attracting significant international interest in the wake of Fukushima. Other priority activities are the development of thermal hydraulics computer codes for predicting the performance of increasingly more passive cooling systems – for both normal and accident conditions – and coupling of these codes to neutronics and structural integrity codes.

ANSWERS codes developments

Over many years, the ANSWERS computer codes have been developed, applied and validated for all the major water reactor systems, including light-water reactors (LWRs) such as PWRs, boiling water reactors (BWRs), VVERs and RBMKs, and also heavy-water reactors such as CANDU. Activities cover operational (reactor physics, fuels), design basis (thermal hydraulics) and severe accident applications. Much of this work carried out for LWR Gen III and earlier generations is relevant to the more novel Gen III+ and SMR designs. ANSWERS codes have undergone extensive V&V (two examples are shown below) and are flexible for modelling these different reactors at different scales.

V&V

Example 1: High burn-up fuel experiments

The ANSWERS codes MONK and WIMS have recently been benchmarked against high-quality radiochemical isotopic assay data published by USNRC for Calvert Cliffs, TMI-1, Vandellós and ARIANE [2]. These data have been acquired from US and international programmes and cover a large range of burn-up. They enable computer code accuracy to be assessed and the uncertainty with code predictions for these conditions to be established.

Table 2 shows percentage errors between calculation and experiment for isotopics for three spent fuel samples from the Calvert Cliffs Unit-1 PWR with uranium oxide fuel, with ~3wt% enrichment. Discharge burn-ups of samples were in the range 27GWd/te to 44 GWd/te and were analysed with WIMS10 with JEF2.2 and JEFF3.1.1 data [3]. The errors are small, within the range 1–12%.

Table 2

Calvert Cliffs analysis [3]: errors (C-E)/E% in g/gU initial

Calvert Cliffs	JEF 2.2	JEFF 3.1.1
Average U	1.21	1.42
Average Pu	4.58	2.39
Average actinide	3.49	2.91
Average FP	12.26	9.28
Average all nuclides	9.50	7.27

Example 2: PWR simulation experiments (DIMPLE reactor)

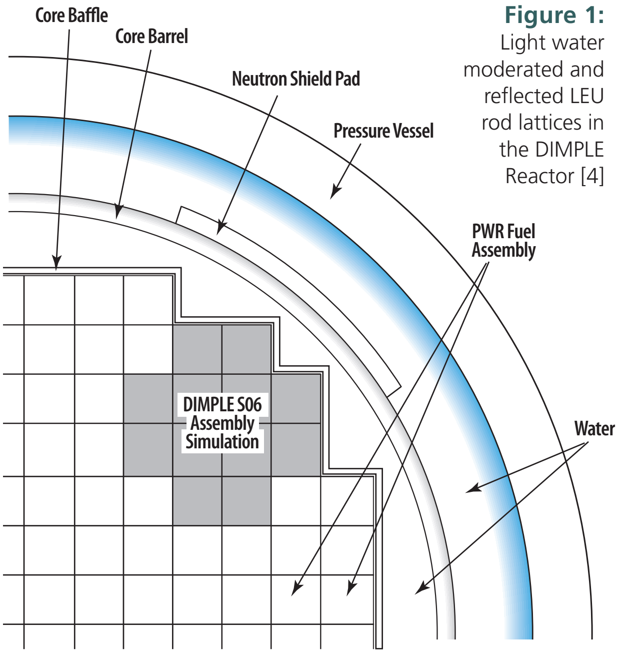

Figure 1: Light water moderated and reflected LEU rod lattices in the DIMPLE Reactor [4]

The ANSWERS reactor physics codes have been validated for PWR conditions against a series of PWR simulation experiments incorporating light-water-moderated and reflected LEU rod lattices in the Winfrith DIMPLE reactor [4]. In particular, the experiments contain geometrical features that make them relevant for small reactors and indeed SMRs.

Experiments were carried out with three variants of the DIMPLE S06 cores: S06A, B and C (see Figure 1). All variants were based on a cruciform array of 3072 3%-enriched uranium oxide pins in water. S06A was a simple cruciform array (12x16x16 pin array) in water. S06B was the same array surrounded by 2.67cm thick steel plates to simulate the steel baffle at the edge of a PWR core. S06C was based on S06B with some fuel pins removed to simulate control rod guide tube vacancies and the addition of boro-silicate glass (Pyrex) tubes to simulate burnable poisons. There were 12 variants of S06C (0–11) with various patterns of vacancy and poison.

Table 3 shows good agreement with experiment of k-effective predictions with the latest versions of WIMS10 with the CACTUS solver using data from the JEF2.2 and JEFF 3.1.1 databases.

Table 3

DIMPLE S06: k-effective comparisons [3]

Core variant	k-effective (JEF2.2)	k-effective (JEFF3.1.1)
S06A	1.00211	1.00325
S06B	1.00068	1.00071
S06C/0	1.00157	1.00166
S06C/8	0.99843	0.99834
S06C/10	0.99905	0.99900
Measured k-effective = 1.0 ± 0.00120		

High-temperature reactors

Technology

High-temperature reactor (HTR) technology offers the potential of higher core outlet temperatures, increased efficiency and applications beyond electricity generation, e.g. process heat and hydrogen generation. For helium-cooled HTRs, there are two basic fundamental core designs: prismatic block and pebble bed.

HTR designs have been put forward from the 1960s to the present day. Early designs were from the UK (DRAGON), Germany (AVR & THTR) and the USA (Peach Bottom & Fort Saint Vrain). More recently, designs for the prismatic type have come from Japan (HTTR), France (ANTARES) and the USA (NGNP); and for the pebble bed type from South Africa (PBMR). Regarding the latest status of HTR, the Chinese HTR-10 is the only HTR that is currently operational, although a larger version (HTR-PM) is under construction.

R&D requirements

R&D is focused on the high-temperature fuel and fuel cycle, materials, the thermal cycle and the balance of plant, in addition to electricity generation, other high-temperature applications (including process heat production) and hydrogen generation. Regarding the fuel and fuel cycle, fundamental HTR (TRISO) fuel is based on uranium oxide particles coated with four layers: porous carbon, a dense inner layer of pyrolytic carbon, a ceramic layer of SiC and an outer layer of pyrolytic carbon. A fuel kernel of UCO with a ZrC layer (in place of SiC) is proposed as an alternative. A thorium (Th) and plutonium (Pu)-based fuel design could also be utilised within a closed fuel cycle.

Design objectives for HTRs are good structural integrity and fission product retention for high burn-up at high temperature. R&D is required to confirm these design requirements. HTR coated particle fuel can be utilised for Pu and minor actinide (MA) management.

ANSWERS codes developments

The ANSWERS MONK and WIMS codes have been developed to model pebble bed modular reactor (PBMR) fuel utilising Monte Carlo and deterministic methods respectively [5]. Thus reactor physics modelling capabilities are available in ANSWERS for modelling advanced HTR pebble bed fuels.

The MONK (Monte Carlo) code models fuel particles within a pebble and the pebbles within the core using algorithms that ensure the correct packing fraction is obtained. This is achieved without having to model partial pebbles or having to accommodate artificial streaming paths, which would not be realistic. Each pebble can have a particular burn-up and this enables the whole core to be modelled.

The WIMS (deterministic) modular code incorporates a triple heterogeneity model to allow for resonance self-shielding. It includes the heterogeneity of the fuel particles, the particles in the pebbles and the pebbles themselves, which can have different burn-up and/or composition. A specific fuel management code capability for the PBMR has been built into the WIMS modelling framework. This enables the model to iterate to an equilibrium core loading. WIMS includes a module to calculate steady-state temperature profiles in PBMR cores. This enables the temperature feedback on cross-sections to be assessed. The initial core would be comprised of unburnt fuel and it would typically incorporate six batches. After each cycle, batch 1 becomes batch 2, batch 2 becomes batch 3, etc.; batch 6 is discharged and batch 1 receives fresh fuel. In principle, it is possible to achieve an equilibrium core burn-up after five iterations, although in practice additional iterations are required to reach an equilibrium k-effective. This is due to some shielding interaction between batches.

V&V

PROTEUS experiments

As part of the International Atomic Energy Agency (IAEA) programme on validation of safety-related reactor physics calculations for LEU [low-enriched uranium] HTRs, PBMR simulation experiments were performed in the Proteus facility at the Paul Scherrer Institute (PSI) (Figure 2). Modelling of different critical assemblies was carried out using the MONK code [6], for representative cores 5, 9 and 10. Analyses of critical k-effective and also the measured shut-down rod (SDR) worth were performed, and results are shown in Tables 4 and 5. Overall, agreement with experiment is good; however, please note that the partially inserted control rods were not modelled, explaining the slight overprediction of k-effective.

Comparisons of MONK SDR worth calculations with experiment are shown in dollars for the representative cores 5, 9 and 10.

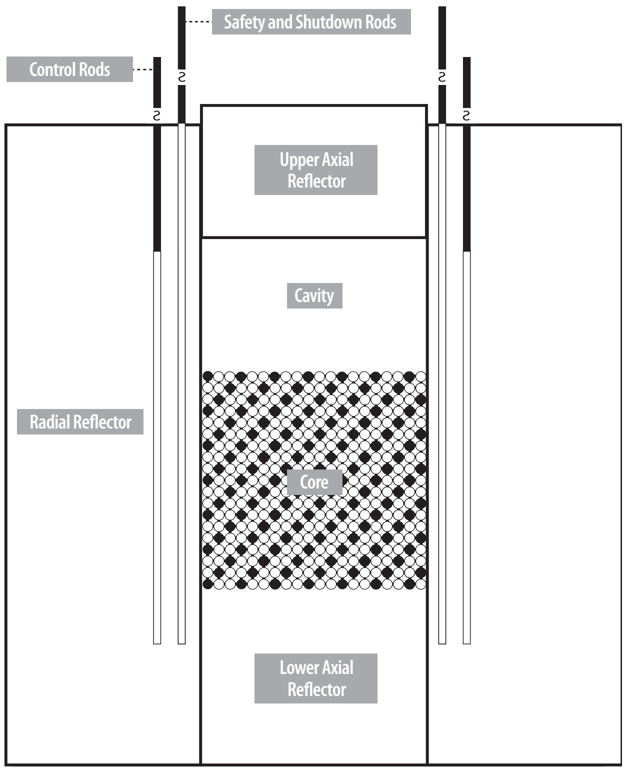

Figure 2: PROTEUS experiments and PBMR modelling using MONK [6]

Table 4			
Results of MONK k-effective calculations for rods withdrawn			
Core	**k-effective**	**One standard deviation**	**Experimental value**
5	1.0112	0.0004	~1.008
9	1.0095	0.0004	~1.008
10	1.0059	0.0004	~1.008

Table 5				
Results of MONK SDR worth calculations, in dollars				
Core	**SDR 5 inserted**		**SDR 5, 6 and 7 inserted**	
	MONK	**EXPT**	**MONK**	**EXPT**
5	-3.45	-3.57	-11.04	-11.45
9	-3.68	-3.68	-11.57	-11.61
10	-2.46	-2.61	-8.20	-8.63

These are generally good, although the results show a tendency to underpredict the SDR reactivity by up to 0.4$. This is approximately proportional to the number of SDRs inserted. It should also be noted that the PSI worths for graphite-filled channels are based on calculation. The statistical uncertainty on the MONK reactivities is 0.08$.

The WIMS HTR models have also been validated against the HTR-10 experiments in China [7].

Sodium fast reactors

Technology

In addition to electricity generation, sodium fast reactors (SFRs) offer sustainable fuel cycle and improved management of high-level waste and spent fuel, possibly including recycling. They can also be used for the management and disposition of stockpiled plutonium from earlier weapons programmes. Much experience of SFRs for electricity generation exists; also, the gas-cooled fast reactor (GFR) offers some advantages over the SFR, combining VHTR and SFR attributes. These are not considered in detail in this paper, although ANSWERS codes have been applied to such systems [8,9].

The SFR has liquid sodium coolant at low pressure but with a higher core power density than the LWRs and the AGRs. SFR designs being considered include: a large loop-type, a medium pool-type and smaller modular design. The SFR concept has been established in various countries for many decades. Prototypes that have successfully operated include: UK (DFR and PFR); USA (EBR I, Enrico Fermi, EBR II and FFTF); France (Rapsodie, Phénix and Superphénix); Russia (BR5, BOR 60, BN 350 and BN600); Japan (Joyo and Monju) and Germany (KNK II). Latest status SFR programmes include: France (ASTRID – SFR demonstrator by the early 2020s) and Russia (BN800 – under construction).

R&D requirements

SFRs require R&D in the development of advanced fuels and potentially MA-bearing fuels, integration of systems, materials and component design techniques. There are operational issues associated with the chemical and physical properties of liquid sodium, and possible safety considerations associated with sodium voidage and neutronic reactivity.

Fuels include mixed oxide for the large liquid sodium designs, nitride and carbide fuels for high-temperature gas-cooled designs, and metal alloy fuels for small modular designs. Issues that require research work include examining the consequences of embedding low thermal conductivity fuel/MA fuel particles in an inert matrix that has higher conductivity. There are various possible fuel cycle options associated with the above processes, around the recycling of highly radioactive fuel and avoidance of the separation of pure plutonium.

ANSWERS codes developments

The ANSWERS codes have been developed for many reactor types, including SFRs. For reactor physics, the MONK Monte Carlo nuclear criticality code, modelling advanced geometry modelling and detailed energy collision treatment, provides realistic 3D models for accurate simulation of neutronics behaviour. It is supported by extensive experimental comparison data for SFR. Similarly, the WIMS reactor physics software package (accommodating the ECCO software for SFR applications) can perform simple pin-cell reactivity calculations up to whole-core estimates of power flux distributions for the SFR.

For fuel performance, the ANSWERS TRAFIC code includes mechanistic models for fast reactor fuel performance in normal operation and fuel response under transient conditions. It has been developed against various fuel-related research programmes, including experimental test programmes such as CABRI, which grew out of the EFR project, and PFR/TREAT. Note that the TRAFIC code is restricted presently to fast reactor applications although some preliminary planning to extend its capabilities to water reactors has been carried out. Other programmes supporting V&V include routine post-irradiation examination, out-of-pile annealing studies of fission gas, and programmes on void swelling under irradiation in neutron and electron beam facilities. Theory and modelling work from other sources (e.g. atomistic modelling of metals and uranium oxide) have also contributed and there have been various OECD/NEA International uranium and plutonium benchmarks [10].

V&V

Zebra experiments

The ANSWERS reactor physics codes have been validated against ZEPHYR, ZEUS and ZEBRA (R&D) in the various stages of their development. Recently, the codes have been validated against various core configurations in the ZEBRA-8 programme at Winfrith, comprised of plutonium metal, mixed plutonium and uranium oxide, and natural uranium oxide plates interspersed with a combination of graphite, stainless steel and sodium plates. Data were obtained for values of k-infinity in a range of thermal, intermediate and fast neutron spectra [11]. These have been benchmarked with MONK (see Table 6), and WIMS incorporating the European Cell Code (ECCO) in the ECCO module. The transport

Table 6						
Comparison of MONK ZEBRA cell k-infinity values with measurement [11]						
Configuration	**Measured**		**Calculated**		**(C-E) pcm**	
	k	1	k	1	(C-E)	1
Core 8/A2	0.9920	0.0063	0.9897	0.0002	-228	630
Core 8/B	1.0010	0.0023	0.9978	0.0002	-325	231
Core 8/C	0.9860	0.0044	0.9786	0.0002	-742	440
Core 8/D	0.9730	0.0045	0.9721	0.0002	-90	450
Core 8/E	1.0060	0.0069	0.9884	0.0002	-1760	690
Core 8/F2	0.9710	0.0042	0.9641	0.0002	-688	420
Core 8H	1.0300	0.0025	1.0349	0.0002	485	251

calculation was carried out by the CACTUS module of WIMS, which solves the neutron transport equation by the method of characteristics (Table 7).

Tables 6 and 7 show good agreement with experiment of k-infinity predictions with the latest versions of MONK and WIMS for configurations with spectra typical of a fast sodium-cooled power reactor. Configurations 8C and 8D, with volume fractions of fuel, carbon and sodium similar to those of a carbide-fuelled fast power reactor, are also well predicted.

Data from the CADENZA configuration in the ZEBRA reactor as part of the International Reactor Physics Experiment Evaluation (IRPHE) benchmarks comparing pin to plate fuel has also been analysed [12]. Other work performed was for the IAEA benchmark for BN600, concerned with the void coefficient for sodium boiling [13]. Various consultancy activities have also been carried out supporting the safety case for removing the breeder elements in the decommissioning DFR and PFR, using WIMS and FISPIN for generation of inventory data.

Advanced fast reactor core design and fuel programmes have included the CAPRA project for plutonium management, and CAPRA/CADRA for MA destruction [14]. The aim is to investigate the use of fast reactors to manage the back-end of the fuel cycle. These programmes have also included gas-cooled fast reactor (GCFR), technology recognising the proven UK gas reactor and LMFR experience. There have also been studies in GCFR systems to reduce the need for heterogeneous MA recycling and EC FP-related programmes.

Table 7			
Experimental and WIMS deterministic benchmark k-infinity values [11]			
Test region	**k-effective Experiment**	**Calculated**	**(C-E) pcm**
Core 8A2	0.9920	0.9852	-696
Core 8/B	1.0010	0.9963	-471
Core 8/C	0.9860	0.9742	-1228
Core 8/D	0.9730	0.9658	-766
Core 8/E	1.0060	0.9805	-2585
Core 8/F2	0.9710	0.9680	-319
Core 8H	1.0300	1.0391	850

Molten salt reactor

Technology

The molten salt reactor (MSR) is the least studied of the Gen IV designs but offers the best conversion ratios, the potential for thorium utilisation and other fuel options. MSRs (Gen IV design) have the unique feature that fuel is dissolved in a liquid salt coolant, typically a mixture of lithium/beryllium fluoride, although lithium/sodium/potassium and sodium/zirconium fluorides are also possible. Other MSR designs have been considered where the function of the molten salt is entirely as a coolant.

Early work on thermal spectrum reactors was carried out at Oak Ridge National Laboratory (ORNL) in the USA during the 1950s and 60s (aircraft reactor experiment, ARE, and the molten salt reactor experiment, MSRE). Regarding fast spectrum reactors, some work was done in the UK, USA (ORNL, ANL) and Switzerland and there was significant work in Russia in the 1970s. No fast spectrum reactors have yet been built but China is developing a thorium-based MSR.

R&D requirements

The chemistry of molten fuel and salt in the reactor technology will be a key area for R&D. The same is true for the fuel cycle, particularly if it involves fuel reprocessing in a closed fuel cycle. There will be operational issues around the fuel and coolant performance in the reactor and the management of gaseous fission product extraction. The safety case will need to accommodate that there may be fewer layers of defence in depth in a molten fuel system.

ANSWERS R&D developments

Work has been carried out in developing ANSWERS codes capabilities in modelling thorium fuel. A Th-232/U-233 thermal breeder core in the US Shippingport light water breeder reactor has been modelled using the deterministic WIMS code and the Monte Carlo MONK code [15]. Study of multiplication factor and depletion included comparison of the thorium data in the latest nuclear data libraries (including ENDF/B-VII, JEFF3.1 and JEF2.2) and revealed significant differences between the libraries. It is an important feature of ANSWERS codes that they are supplied with multiple nuclear data libraries allowing the user to compare the results from different evaluations, such as the European (JEFF), US (ENDF/B), Chinese (CENDL) and Japanese (JENDL) libraries.

V&V

The CRITEX code has been developed to model criticality in fissile solutions with cylindrical geometry. It was developed jointly with CEA and has been validated against the French CRAC and SILENE [16] and Japanese TRACY [17] experiments. Through ANSWERS association with Imperial College we have also been involved in work with their FETCH code, which is a coupling of three-dimensional transient neutronics with their FLUIDITY CFD code [18]. This can be used to model fissile solution reactors of arbitrary geometry [19].

Conclusions

The ANSWERS radiation transport codes have been developed over the last 50+ years for a very broad range of applications and have undergone very extensive V&V. The physics scope includes nuclear criticality, reactor physics, radiation shielding and dosimetry applications, including thermal hydraulics, structural and other feedbacks.

Applications cover reactor operations safety and performance, fuel and waste management facilities, transport of nuclear materials, and repository design and sustainability. All scales can be modelled: research reactors, prototypes, SMRs, large power reactors and reactors for other energy applications. Types of reactors modelled include: LWRs (PWR, BWR, VVER, RBMK), PHWRs (CANDU), HTRs, FBRs and liquid fuel reactors, and current designs and future (including Gen IV) concepts are considered.

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Peter Smith is a senior reactor physicist in Amec Foster Wheeler; he is also applications lead for the WIMS code which is used for reactor physics analysis in the UK and worldwide. This includes the modelling of a wide range of thermal, fast and advanced reactor types including PWR, BWR, SFR and HTR systems.

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