Status and perspectives of ASTEC models

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SUMMARY

During the 4 and a half years of SARNET, 30 partners have assessed the ASTEC V1 European integral code successive versions through validation, i.e. comparisons with results of experiments, and benchmarks with integral and/or mechanistic codes.

Validation tasks on about 65 experiments were performed to cover all physical phenomena occurring in a severe accident: circuit thermalhydraulics, core degradation, fission products (FP) release and transport, Molten-Corium-Concrete-Interaction (MCCI), in the containment, thermalhydraulics, aerosol and iodine as well as hydrogen behaviour. In parallel, IRSN and GRS have applied the models under development to other experiments: some results are very promising, in particular for iodine behaviour on Phebus.FP and ISTP experiments (such as EPICUR). The overall status of validation can be considered as good, with results often close to results of mechanistic codes. Some reach the limits of present knowledge, for instance on MCCI where latest results will be presented. And like in most codes, an adequate model for reflooding of a degraded core is still missing, in particular as regards the corresponding strong hydrogen release.

As to ASTEC benchmarking, about 20 benchmarks with other codes on plant applications were performed for diverse reactor types (PWR 900, Konvoi 1300, Westinghouse 1000, VVER-1000 and VVER-440) and scenarios (SBLOCA, MBLOCA, LBLOCA, Loss of Steam Generator Feedwater and SBO). The main orders of magnitude and trends of results, which is the crucial aspect for integral codes, are similar to MELCOR or MAAP4 results. Good results are as well obtained on comparison with mechanistic codes such as ATHLET-CD, ICARE-CATHARE and RELAP5-3D. In particular, many benchmarks on RCS thermalhydraulics with CATHARE2 reference code were done by IRSN with good results.

The latest V1.3rev2 version was released in Dec.07 to all partners. It is currently the reference version for the IRSN PSA2 on French PWR 1300 MWe and for the GRS PSA2 consolidation study on Konvoi-1300 MWe. In parallel, IRSN and GRS are preparing the new series of ASTEC V2 versions that will account for the needs of evolution expressed by the SARNET partners. The 1st version V2.0, planned for March 09, will be applicable to EPR and will include the ICARE2 IRSN advanced core degradation models. Beyond, the scope of application for the next versions will extend to BWR and CANDU reactors where the needs are mainly limited to the phenomena occurring during the core degradation phase.

ASTEC will continue to play a key role in the SARNET2 network, as a repository of generated knowledge through new or improved models.

A. INTRODUCTION

The ASTEC (**A**ccident **S**ource **T**erm **E**valuation **C**ode) latest version V1.3rev2 was released by IRSN and GRS in December 2007 to the partners of the ASTEC Topic. It is currently the reference version for the IRSN Probabilistic Safety Assessment (PSA2) on French PWR 1300 MWe and for the GRS PSA2 consolidation study on Konvoi-1300 MWe. Twenty-five partners (see Table 1 below) have assessed this version in 2008 through validation against experiments and benchmarks with integral and/or mechanistic codes.

Table 1: ASTEC Topic partners in SARNET 4th year

AECL (Canada)	ARCS (Austria)	AREVA-NP (France)	BUTE (Hungary)
CEA (France)	CIEMAT (Spain)	EA (Spain)	EDF (France)
ENEA (Italy)	FZK (Germany)	GRS (Germany)	IKE (Germany)
INR (Romania)	INRNE (Bulgaria)	IRSN (France)	IVS (Slovak Rep.)
JRC-IE (EC)	JSI (Slovenia)	KTH (Sweden)	LEI (Lithuania)
NRG (Netherlands)	TRACTEBEL (Belgium)	TUS-EI (Bulgaria)	UJD (Slovak Rep.)
UJV (Czech Rep.)	VEIKI (Hungary)	VUJE (Slovak Rep.)	

This work has completed the assessment done during the three first 12-months periods, leading to a total of about 65 different experiments covering all physical phenomena involved in SA. The benchmarks on plant applications have concerned diverse reactor types (PWR, VVER and BWR) and SA scenarios in operation states.

In parallel, IRSN and GRS are currently preparing the new V2 family of versions that will account for the needs of evolution expressed by the SARNET partners during the 4,5 past years. The 1st version V2.0, planned for March 09, will be applicable to EPR and will include the ICARE2 mechanistic models for core degradation.

B. STATUS OF ASTEC V1 CODE

Since many years, the ASTEC code, with its versions V0 then V1 that have integrated continuously the progress of international knowledge, has been applied as a reference code to important IRSN safety studies, for instance:

- Review of the source term on French reactors through detailed analysis of reference SA scenarios,
- Design of the recombiners implemented in the French PWRs,
- Fission product (FP) distribution for evaluation of the equipment behaviour in a PWR containment.

The V1 versions are being intensively applied in the frame of the IRSN PSA2 on 1300 MWe reactors. Many different scenarios are being analysed, including operation of the safety systems: LOCA (Loss of Coolant Accident), SBO (Station Black-Out), LOFW (Loss Of Steam Generator Feedwater), SGTR (Steam Generator Tube Rupture)….

A specific project started in 2007 at GRS to consolidate the code applications for PSA2 on Konvoi 1300 reactors: benchmarks are being performed on various scenarios with the MELCOR code with a focus on the evaluation of the source term.

The number of users throughout the world reaches now more than 90 qualified scientists. The version can simulate all types of scenarios for PWR and VVER reactors in operation states, taking almost all phenomena into consideration, except late reflooding of a degraded core and air ingress (steam explosion has always been out of the scope of the code). All models are at the current State of the Art, except the model of reflooding of a degraded core that is still inadequate (like for most codes). The level of validation is very high for most phenomena, especially the FP behaviour and the Reactor Coolant System (RCS) thermal-hydraulics. In particular, the syntheses of interpretation of all Phebus.FP integral experiments rely strongly on the ASTEC modules. Several benchmarks with the CATHARE2 French reference thermal-hydraulics code on diverse scenarios in PWR 1300 showed a good agreement.

As to safety systems and Severe Accident Management (SAM) for the existing PWR and VVER, all can be represented, except the reflooding of strongly degraded cores: e.g. volunteer primary circuit depressurisation, SG management, spray system and venting in the containment.

As shown in ERMSAR-07 [1], ASTEC V1 is fully applicable to all VVER. The first applications to BWR and CANDU reactors show that all models are already applicable except for core degradation up to vessel (or calandria) failure.

C. OUTCOMES OF ASTEC V1 ASSESSMENT IN SARNET

Large validation efforts have been devoted during the 4,5 SARNET years: about 65 different experiments have been analysed. The conclusions, globally satisfactory, are summarised in 2 ERMSAR-08 papers: one on primary circuit thermal-hydraulics and core degradation [2] and the other one on FP behaviour [3]. In particular, the good present level of FP models allows to evaluate with more details the source term, as underlined by the gas chemistry complex models. For containment models, the results were globally good, as shown in an ERMSAR-07 paper [4]. For MCCI, progress is accompanying the large international R&D, as shown by IRSN first attempt to build a comprehensive view of real material experiments in homogeneous corium configurations (OECD-CCI, VULCANO) and different concrete types (siliceous, sand-limestone) [5]. This interpretation is promising but the models are not yet fully predictive. There is the need of new experimental data and of progress of understanding in SARNET2 and OECD-CCI frame.

The main ASTEC V1 weakness remains the models of core reflooding where the models remain inadequate, like all codes, in particular for strongly degraded cores. For a real progress, there is the need of magma-debris ICARE2 models in ASTEC V2 as underlined by the benchmark with ICARE/CATHARE V2 (see below). Another (less important) weakness concerns Direct Containment Heating (DCH) for present reactors, where needs of improvements have been identified.

Twenty-seven plant applications were performed in 2008 on PWR900-1300, Konvoi1300, West.1000, VVER-1000 and VVER-440 reactors, eleven calculations including all modules. Various scenarios were analysed: LOFW, SBO, LOCA (SB, MB, LB), SGTR. The numerical robustness can be today considered as good, as confirmed by the numerous calculations currently done for the IRSN PSA2 on PWR 1300 MWe. For computation time, the results are variable but ASTEC runs roughly close to real time.

The latest benchmarks done with V1.3rev2 confirm what was already presented at ERMSAR-07 [1]. With the integral codes MELCOR and MAAP4, the trends and the orders of magnitude of the main sequence results are comparable. The agreement is good on RCS thermal-hydraulics, hydrogen in-vessel production (kinetics and total mass), containment behaviour, MCCI (the latter underlined by the stand-alone benchmark for a VVER1000). Note that the agreement on kinetics of hydrogen production is much better than with previous ASTEC versions. But some differences, obviously related to differences in physical models, in particular for core degradation (in ASTEC: 1D candling of molten mixtures along the rods), remain on the following results: kinetics of core degradation and thus on lower head failure time (but with a difference staying below 20%); FP/aerosol release from core and retention in RCS. With the mechanistic codes such as ICARE/CATHARE V2 (IRSN) or ATHLET-CD (GRS) for RCS thermal-hydraulics and core degradation, the agreement is good on RCS thermal-hydraulics, in-vessel hydrogen production (mass, kinetics), corium masses in lower plenum and lower head failure time. Note that these above results are crucial for a PSA2, which allows ASTEC V1 current applications to PSA2 or safety studies. But differences are observed on core degradation kinetics due to magma 2D relocation ICARE2 models: these models lead to a larger radial corium relocation in the core and a later slump in the lower plenum than the candling models (Figure 1). Indeed, the detailed timing of events during the core degradation is more realistic with the 2D magma relocation models, which is important for the management of the accident.

Note that two participants of the OECD/NEA benchmark exercise on a TMI2 alternative scenario have used CESAR-DIVA. Their results were in good agreement with other codes, which confirmed that ASTEC has reached a satisfactory level of confidence for such reactor applications, with respect to other internationally used codes. Besides, these independent applications gave very consistent results, which proves the code reliability.

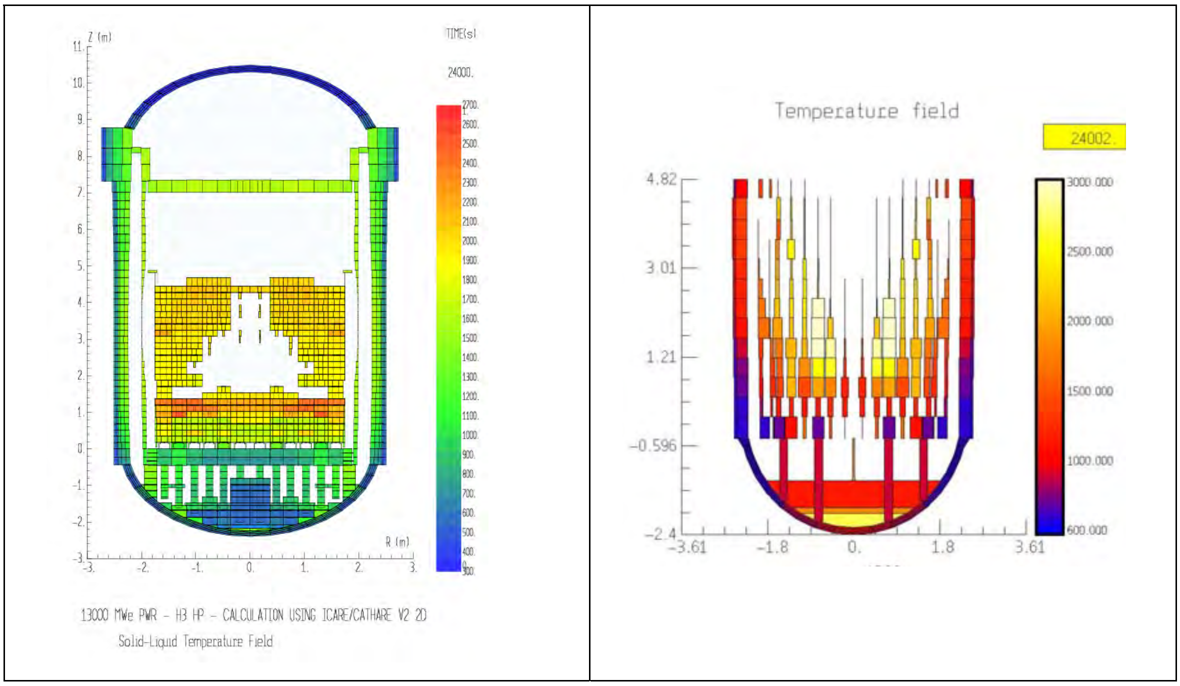

Figure 1 : Comparison of calculated core states at time of vessel failure between ICARE/CATHARE V2 (left) and ASTEC V1.3 (right) for a SBO on PWR 1300 Mwe

The ASTEC capability to simulate In-vessel Melt Retention in case of vessel external cooling was demonstrated in the ERMSAR-07 paper [6] in the VVER-440 case. More detailed models will be available in ASTEC V2.

E. ASTEC V2 PLANS AND PERSPECTIVES

IRSN and GRS have released the plan of development accounting for the SARNET users' needs as expressed in the SARNET report released end of 2006. The 1st version V2.0 is currently under preparation and should be released in March 2009, including significant model improvements such as for instance: most core degradation models from ICARE2 (in particular in-vessel 2D magma-debris relocation), ex-vessel EPR corium catcher, and some FP new models such as Ruthenium behaviour in core and containment and kinetics of iodine chemistry in RCS gas phase. The model adaptations to other reactor types than PWR are described in the ERMSAR-08 paper in [7], including the adaptations to the EPR. All other “generic” model improvements or new models are described in the following paragraphs, along with the corresponding plans for validation.

E.1 Main V2 models for RCS thermal-hydraulics and core degradation

RCS thermal-hydraulics

The priority is the operation in reactor states at low pressure, e.g. shutdown states or mid-loop states. Tests on the ASTEC V1/CESAR module are ongoing but a priori no large adaptation of models seems necessary. The validation will be done by comparison with available CATHARE2 results. In parallel, the model of non-condensable gases is extended to any number of gases (only one non-condensable gas in V1). This will give several advantages: at short term, manage without any numerical difficulty the situations of total oxygen starvation that may occur during a scenario; on a longer term, to be able to model in-core air flows for clad oxidation after air ingress into the vessel, and to allow future applications to circuits with any gas (either experiments or High Temperature Reactors).

For high-pressure scenarios, the failure times of the RCS components (main cooling line, surge line, steam generator tubes…) should be evaluated, accounting for the walls temperature gradients and the temperature-dependent material properties for plasticity and creep. In a first stage, analytical models, already available at IRSN, will be implemented.

In a longer term, the CESAR models will be extended to simulate 2D two-phase flow patterns in the core region, i.e. cross-flows above the water level and natural convection loops. This evolution is closely linked to the change of coupling method between thermal-hydraulics and core degradation with respect to the ASTEC V1 method (see below): ICARE2, differently from DIVA, will be no more in charge of modelling thermal-hydraulics in the core but only the interactions between materials and the corium formation and relocation.

Core degradation

The ICARE2 IRSN mechanistic code for core degradation will be the ASTEC V2 module, replacing the ASTECV1/DIVA one. In particular, it will include the following models:

- First, what is the most important progress, the models of 2D relocation of molten corium and debris. These models are based on a porous media approach**.** They are more realistic than the V1 models 1D of candling relocation along the rods since they allow reproducing the formation of the in-core corium molten pool and the corium relocation through the complex core lateral and lower structures as it happened in TMI-2 accident. The magma oxidation is modelled. All these models have been very intensively validated in the past years in the frame of the ICARE/CATHARE International Users Club [8].
- Radiative heat transfers in the core. An "equivalent radiative conductivity" approach in a porous medium is used (Figure 2), more physically reliable than the former model from ASTEC V1 and applicable in continuity along the evolution of degradation of core geometry, from the intact bundles up to the molten pool and the debris beds. This model will be extended to account for a semi-transparent medium, with absorption by steam and droplets.
- Steam oxidation and creep behaviour of Zr1%Nb claddings typical of present VVER cores.
- Detailed behaviour of the main lateral and lower structures, such as core support plates, in order to represent precisely the in-vessel real geometry and their effect on corium slump into the lower plenum (additional steel mass, delay on the slump, etc…).
- Corium behaviour in lower plenum. The simplified fast-running ASTEC V1/DIVA model with 0D corium layers (oxide corium, metal corium, debris) will be kept but stratification models are being added, based on the interpretation of the MASCA RRC-KI experiments (done in the frame of the OECD project): the Figure 3 illustrates good preliminary results despite equilibrium seems to be reached too quickly On a longer term, a more mechanistic model will be developed, accounting for species transport by turbulent convection. Validation will be based on the past experiments FOREVER (KTH), RASPLAV and MASCA (RRC-KI) and on the on-going and future ones in LIVE (FZK).

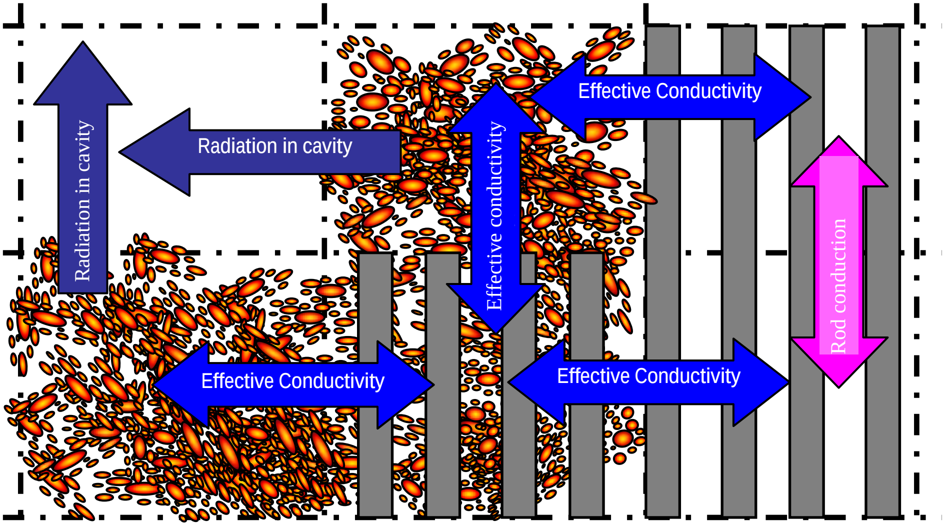

Figure 2 : ICARE2 model of radiative heat transfers in the core region

As written above, the reference model for corium relocation will become the 2D magma-debris model. But the candling 1D model will be kept for a unique situation where it is better adapted: the flow of molten mixtures within the gap between the cladding and the guide-tube of control rods (such as SIC ones) that follows a 1D pattern.

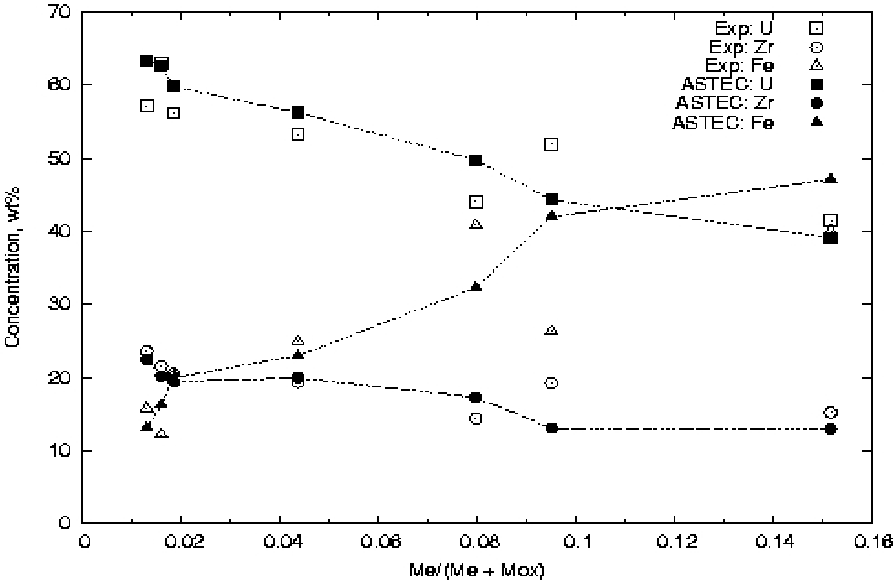

Figure 3 : Validation of ASTEC V2/ICARE2 on MASCA experiments

For situations of reflooding of quasi-intact cores, still in bundle geometry, the existing ASTECV1/DIVA model seems sufficient in a first stage, at least for bottom reflooding: it was validated on PERICLES (CEA) and QUENCH (FZK) experiments. Later on it will be adapted to the future CESAR core 2D thermal-hydraulics. However, modelling of reflooding of a degraded core (corium pool, debris and remnants of fuel rods) remains a big challenge for any code and large R&D efforts are now planned in SARNET2. In a first stage, an attempt to get a simplified model will be done but most efforts will focus on a more mechanistic model for the longer term (perspective of 2011-2012), based on the current ICARE/CATHARE V2 models and in close relation with ongoing experimental programs on debris coolability in SARNET2 (in particular the IRSN PEARL program currently under design). Note that this detailed model will need the CESAR 2D thermal-hydraulics both in the core and in the lower plenum.

For the mechanical rupture of the vessel lower head, the ASTEC V1 "OEUF" model seems adequate and validated enough (on LHF/OLHF experiments in SNL and on FOREVER ones in KTH) for evaluating the time and location of rupture for PWR vessel hemispheric shapes. The LOHEY alternative ICARE2 model being adapted to the ellipsoid shape of most VVER, both models will coexist in ASTEC V2. Later on some improvements of the existing ASTEC models could come from failure surfaces determined from numerical simulations of LHF/OLHF experiments and accounting for different reactor steels.

For air ingress after vessel lower head failure, a preliminary model is today available in ICARE2 for enhanced clad oxidation and loss of rod integrity, but it will only be operational once the CESAR extension to core thermal-hydraulics and to any number of non-condensable gases is done. Improvements are planned to account for the transport of oxygen and nitrogen in the oxide layer and in the cladding layer metal, the interaction between oxygen, nitrogen and the metal and also the impact of oxides and nitrides on cladding mechanical states.

Coupling between in-vessel thermal-hydraulics and core degradation

A new coupling method is being defined by IRSN on the basis of the ICARE/CATHARE V2 approach. Preliminary testing started in late 2007. This new approach is globally similar to the one used in ICARE/CATHARE V2 IRSN code, as well as in the GRS ATHLET-CD code. It assumes distinct roles for the 2 modules: one, CESAR, dealing with thermal-hydraulics in the whole RCS (i.e. the vessel and the loops), and the other, ICARE2, dealing with core degradation, i.e. materials evolution and relocation. The advantage will be to replace the V1 coupling method, where the switch from CESAR to DIVA had some drawbacks: complexity for the developers, complexity for the user, and sensitivity in case of violent event such as accumulator discharge. The use of a unique thermal-hydraulics in the whole RCS would also have the advantage, in case of late in-vessel reflooding, i.e. water injection into a degraded core (corium molten pool, debris, remnants of rods...), to be able to totally fill up the RCS loops with water, up to a stable core configuration, which was not possible with the V1 method. The method adopts a prediction/correction approach. It consists in decoupling the time-steps of each module, thus allowing the use of relatively large time-steps due to the larger time-step for the core degradation module (around 1s.) while the thermal-hydraulic module may run, if necessary (in particular for situations expected with 2D thermal-hydraulics), with a much smaller time-step. This method applies too in presence of chemical reactions that modify the fluid composition. It warrants the exact mass and energy conservation whatever the time-steps, the only condition being that the core degradation time-step represents a meeting point for the thermal-hydraulic module.

E.2 Main V2 new models for ex-vessel corium behaviour

Direct Containment Heating

The necessary improvements with respect to ASTEC V1, including scaling up for plant conditions, have been identified:

- More general thermal-hydraulic models for gas flows between reactor pressure vessel (RPV) and cavity, with possibly the implementation of specific mass/energy flow equations,
- Better modelling of flow paths and particle distribution through dedicated correlations for specific reactor type cavities and containments.
- Better modelling of corium oxidation in cavity and in the containment zones.

They will have to be specified in details in 2009. But the general principle is to keep the ASTEC V1 general structure globally unchanged in V2, thus keeping a specific module RUPUICUV. Another improvement will consist in the integration into the CPA module of the models for transport and behaviour of hot corium droplets entrained by DCH (today modelled in ASTEC V1 with the simplified parametric CORIUM module).

MCCI

A first model evolution in the MEDICIS module concerns radiative heat transfers in the cavity semi-absorbent atmosphere (containing steam, carbon dioxide or concrete aerosols). Besides, the thermal behaviour of the cavity upper lateral walls can also now be described in details, up to melting of concrete. Unfortunately, no available experiment being available for a detailed validation of such models, only parametric calculations will be performed.

Model improvements will be directly issued from the feedback of the continuous interpretations of international experiments (OECD-CCI in ANL, VULCANO in CEA, future experiments in the frame of the International Science and Technology Centre or ISTC), either with real materials or with simulant ones:

- Phenomenological models deduced from the above experiments,
- Heat exchange coefficient as a function of local gas bubble velocity,
- Evolution of pool void fraction as a function of local gas bubble velocity,
- New model for metal/oxide heat transfer based on ABI experiments (done by CEA in the 3-parties CEA-EDF-IRSN frame) and on a series of simulation results obtained with mechanistic codes (such as heat transfer calculations with bubbles crossing a liquid/liquid interface for reactor conditions),
- Distribution of convective heat transfer coefficients along the pool/concrete interfaces, based on CLARA analytical experiments (done by CEA in the 3-parties CEA-EDF-IRSN frame),
- New criteria for pool configuration switching, based on the use of mechanistic simulation codes.

For FP and aerosols release in MCCI (not modelled in ASTEC V1), models have been implemented in ASTEC V2 and validated on the ACE experiments (ANL in USA). The 1st one uses the thermo-chemical model from the ASTEC V1/ELSA module for FP vapour pressure computation and assumes that vapour transport is driven by gas bubbling. The 2nd one on aerosols release uses an empirical correlation defined by IRSN from the interpretation of the ACE experiments.

For heat conduction in the concrete basemat, a simplified analytical model (and fast-running) will be implemented in the short term on the basis of open literature. In a longer term, the extension to multi-D effects will involve the extension of the cavity erosion algorithm and the account for 2D heat conduction (or even 3D) across the basemat should aim at a more realistic modelling of the corium cavity evolution in the long-term MCCI phase, particularly the energy sinks due to heat losses by conduction. This would imply the addition of concrete meshing and of one heat balance equation in the concrete basemat.

For concrete and thermo-chemistry models, the existing V1 models will be extended:

- Literature review on concrete behaviour under decomposition and ablation, and associated modelling improvement,
- Addition of oxidation reactions (production of gaseous SiO),
- Extension of the MEDICIS interface with the GEMINI2 thermodynamic solver to 3 poles (initial corium, oxidized metals, concrete oxides) and of the tabulation approach carried out in MEDICIS (the latter approach being the only one available for any ASTEC partner). More than 3 poles will be considered if several concrete types are involved.

E.3 Main V2 new models for fission product behaviour

FP release from the core

The plans are a continuous improvement of the models of the ELSA module in close link to the interpretation of experiments, in particular in SARNET and in the frame of the International Source Term Program (ISTP):

- Semi-volatile FP release (Eu, Sr, La, Ce and Ba), with validation on the VERCORS (CEA) and Canadian (AECL) experiments,
- UO_2 oxidation by air and reduction by H_2, with validation based on the VERCORS and AECL experiments.
- Release from SIC (Silver-Indium-Cadmium) alloys in PWR control rods. The model improvements will be based on the ongoing interpretation of EMAIC (CEA) and QUENCH-13 (FZK) experiments in the frame of the SARNET interpretation circles. This work should answer the remaining questions concerning the release rate as a function of pressure at the cladding rupture and the characteristics of the subsequent mixture candling. The work will also rely on a review of thermodynamic data (activity coefficient, partial pressure) on AIC-Zr(O) system that is carried out in 2008 in the frame of a IRSN collaboration with CNRS/TECSEN in Marseille.
- Release of FP and structure materials from the corium pool in the vessel lower plenum, with validation on the EVAN Russian experiments (ISTC frame) and the MASCA and MASCA2 experiments (RRC-KI).
- UO_2 volatilisation model, based on the VERCORS RT (CEA) and AECL experiments under air conditions.

The model adaptation to MOX and high BU fuel should mainly consist in the adaptation of the existing correlations, on the basis of available experiments (VERCORS RT, VEGA at JAERI and in future VERDON at CEA and VERONIKA in ISTC frame) and of a literature review.

A new model has been developed for Ruthenium release from the core in oxidising conditions. The results of validation on the Canadian UCE12, HCE1 and HCE3 experiments (AECL) are good on kinetics of release and total released fraction.

FP transport in the RCS

The main new model is kinetics of chemical reactions involving iodine in RCS gas phase. The preliminary application of the ASTEC V2 development version to Phebus FPT1 gives very promising results (Figure 4): this calculation shows a fraction of gaseous iodine at RCS exit, like in the experiment, while the ASTEC V1 equilibrium chemistry model only calculates iodine under the aerosol form at this same location. This model will indeed need further validation on the new IRSN CHIP experiments presently done in ISTP frame.

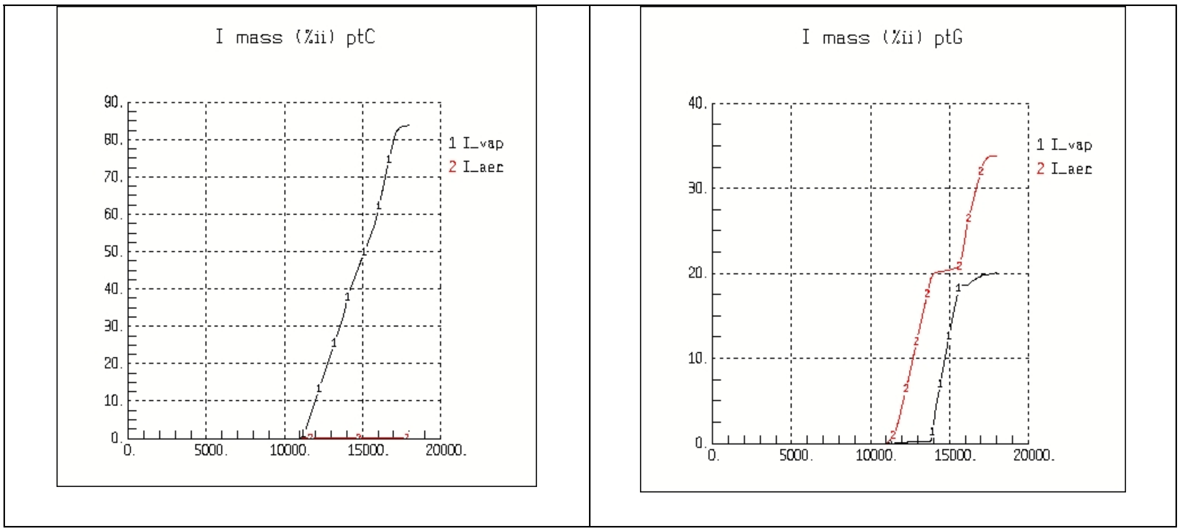

Figure 4 : Preliminary ASTEC V2 results of new iodine chemistry kinetics model on Phebus FPT1 (point C: upstream SG at 700°C; point G: downstream SG at 150°C)

Another new model concerns aerosol trapping in the secondary side of flooded SG. It has been developed on the basis of the ARTIST experiments (PSI). For retention in the SG dry secondary side, a simple model will be developed. It will be based on future detailed computations, using CFD (“Computational Fluid Dynamics”) or LES (“Large Eddy Simulation”) approaches, and validated on the ARTIST program.

For Ruthenium transport and behaviour in RCS, the implementation of a more adequate model than in ASTEC V1 (possibly for instance a kinetic equation) is planned in collaboration with VTT, with further validation on AEKI experiments.

The other module evolution concerns improvements of existing models:

- Aerosol mechanical resuspension, due for instance to some events such as steam explosion or core reflooding. Work is ongoing to improve the actual rock’n roll model, in the SARNET frame in collaboration with Newcastle University but also through a PhD thesis in collaboration with the Ecole Centrale de Lyon (France) and with PBMR Ltd. (South-Africa). Validation is expected in the next years in the frame of this thesis on PBMR experimental data.
- Revaporisation of aerosols, due to chemical changes in aerosol deposits induced by the evolution of thermal-hydraulic conditions such as air ingress in the circuit or re-heating of walls. This process is being investigated in SARNET frame. The proposed modelling will be validated on VTT and VERCORS HT experiments (where some revaporisation was observed during the transients) and possibly on CHIP future ones.

FP behaviour in containment

Several model improvements are planned in the IODE module as possible feedback from ongoing experimental programs:

- Improvement of the modelling of RI formation in the gaseous phase, taking into account humidity, from EPICUR (IRSN in ISTP frame) and OECD/BIP Canadian experiments,
- New model for evolution of pH in the sumps,

- Improvement of the modelling of I_2 adsorption/desorption from paints based on OECD/BIP experiments,
- Introduction of a simple modelling of iodine aerosols interaction with paints, leading to release of volatile iodine (I_2), depending on the state of the paint (dry or wet). Validation should be done on future EPICUR experiments,
- Introduction of the I_2 – CH_4 homogeneous reaction, based on literature data and checked on the Phebus FPT3 experiment.
- Modelling of Ruthenium behaviour in the containment, based on the EPICUR experiments. New chemical reactions were introduced in the V2 development version for decomposition of RuO4(g) coming from the RCS and for production of RuO4(g) in the containment by Ru deposits oxidation. A preliminary plant application has shown the potential impact of Ru on source term.

A new module, DOSE, is being developed for dose rate evaluation in containment gas phase, for use in most of the IODE gas phase chemical reactions. Validation is performed versus detailed computations with the MERCURE/MERCURAD dedicated IRSN codes.

Some new models, missing yet in ASTEC V1, are planned too:

- Formation and destruction of iodine oxide species, with possible validation on EPICUR and ThAI (at Becker Technologies in Germany) experiments,
- Aerosol chemistry, consisting in a more detailed and complete modelling of the abovementioned iodine aerosols interaction with paints,
- Introduction of the influence of impurities in the liquid phase liquid on the iodine volatility (reaction with iron hydroxides or with silicates), based on the ISTC/EVAN findings.

E.4 Main V2 new models for containment

The following improvements of existing models in the CPA module are planned:

- Thermal-hydraulics through the leakages in the containment walls, based on IRSN analytical experiments under way and on experiments done on the PLINIUS CEA platform in SARNET frame,
- Aerosols retention in the leakages in the containment walls, based on IRSN analytical experiments under way,
- Pool scrubbing (SPARC-B models) from the COCOSYS improved GRS model, with validation on POSEIDON or Spanish experiments available in SARNET.

The only new model that is planned at short term deals with the effect of hydrogen combustion or steam explosion on resuspension of deposited aerosols: it will be transferred from the COCOSYS GRS code. Beyond, other future model improvements may concern recombiners (based on OECD-ThAI experiments), FP release from pools and sumps (wet resuspension modelling). In particular, interactions of catalytic recombiners with iodine aerosols should be modelled; validation would take place on the experiments planned in the OECD ThAI project.

For the safety systems, the model of ice condensers, present in some PWR (Loviisa VVER-440 in Europe and some US PWRs), will be transferred from the COCOSYS code.

For gas combustion, the trend is to focus on 3 models (the DECOR model implemented in CPA in ASTEC V1 will not be kept):

- AICC (Adiabatic Isochoric Combustion Calculation) envelope evaluation of pressure peaks,
- Fast-running evaluation using the COMB parametric model from ASTEC V1, but with the improvement consisting in using the flame front propagation model for estimation of the combustion time needed by the COMB calculation (given by the user as input in ASTEC V1).
- For a more detailed analysis of slow and fast turbulent deflagration processes, if acceleration criteria are met, a series of PROCO model calculations varying the ignition time and position.

In the two latter solutions, an extensive validation will be required (e.g. RUT, ENACCEF, ThAI, NUPEC….) to define the limits of the correlations and the code user guidelines.

E.5 Users 'tools

Material data bank (MDB)

All material properties will be progressively gathered in the MDB library. The objective is to obtain an international reference databank and to couple it thoroughly with ASTEC. In ASTEC V1, MDB is systematically used in the modules ELSA, SOPHAEROS, MEDICIS and IODE. The extension of its use in CESAR, ICARE2 and CPA will be done step by step.

The databank will be continuously reviewed and improved, accounting for the evolution of knowledge, in particular for chemical species properties. For the condensed phase chemistry, numerous data on Gibbs functions are missing (liquid/solid); an update of data is necessary. Similarly, there is a need of update of surface tension data used for homogeneous nucleation of chemical species (by default, when the data is missing, the UO_2 surface tension is applied), of viscosities and of emissivities. The update of data on SIC alloys will also be integrated.

The MDB improvements will rely on the continuous improvement of the NUCLEA European thermodynamic databank [9]:

- For thermochemistry, most of MDB data result from NUCLEA (or the associated MEPHISTA databank);
- For corium properties (liquid fraction, enthalpy…), either some result directly from NUCLEA data, like the thermodynamic part of the ICARE2 corium pool model, derived from the U-O-Zr-Fe NUCLEA phase diagram; or an approach of tabulation was adopted on basis of NUCLEA data, for instance for MEDICIS ex-vessel corium (there is today a size constraint on the number of elements for this tabulation approach).

SIGAL-ODESSA tool

The SIGAL-ODESSA tool is the basis of the ASTEC structure around its dynamic memory database. The new ODESSA-MP version will allow the code use in parallel software environments and thus accelerate the ASTEC computations. The objective is, through the use of multi-threads PC, to parallelise the run of each module during a macro-time step. No generalisation to the parallel run of each module, e.g. using a PVM-type tool, will be investigated since it would too much modify the code structure. A factor of 2.5 was gained with ODESSA MP on CESAR computing time without any programming efforts; investigations will go on to reach an overall factor of gain by 5. This will be useful in the longer-term perspective of ASTEC V2 use for emergency response tools or for simulators extended to severe accidents.

Users' tools

In a first stage, two types of users’ tools will co-exist:

- On one hand, diverse tools within the ODESSA package: first the ASTEC V1 tools such as visualisations (on-line and post-processing) and GTIC post-processing; secondly a new pre-processing tool, JADE, allowing the user to automatically and easily check the input decks with the help of graphic pictures;
- On the other hand ATLAS [10] for post-processing of ASTEC results in Windows environment. The objective will be to provide each user with a basic graphic file for each type of reactor.

In a second stage, a combined use ATLAS-JADE will be investigated for easy generation of graphic files. An ATLAS on-line version will be prepared for a long-term use in simulators, with user-interactions during a calculation, e.g. switching of pumps or valves.

The code coupling with uncertainty tools will make easier the users' work to study the influence of uncertainties on input data or models. Such coupling has been made operative in 2008 with the SUNSET IRSN tool.

Documentation

The code documentation will be kept complete and up-to-date: the main efforts in priority will concern in 2008 the update of the whole CPA documentation and of the ICARE2 physical description.

The documentation format will be as homogeneous as possible. Progress is expected to get dynamic hyperlinks that would allow the user to get either a rapid overview of the code content or easily to focus on one part of the code. It will also allow the user to switch from a description of a theoretical model to the description of the corresponding input data and to an example of input deck. Besides, particular care will be given to the Users’ Guidelines that is an essential document for the users.

E.7 Time-schedule of versions

Three versions are foreseen in the next years:

- **V2.0, to be released in March 2009**, roughly at time of start of the SARNET2 follow-up, mainly including ICARE2 advanced core degradation models and applicable to the EPR.
- **V2.1, to be released mid-2010**, mainly characterised by a new coupling approach between RCS thermal-hydraulics and core degradation and by the full capabilities for shutdown states, vessel external cooling and air ingress situations.
- **V2.2, to be released end of 2011**, constituting an international reference version, integrating a large part of the knowledge generated in SARNET, SARNET2 and ISTP, and first version applicable to the major part of BWR and CANDU sequences.
- Beyond 2011, no precise plan can be reasonably done now but a 4th version **V2.3 could be released in 2013**, integrating the whole SARNET2 and ISTP knowledge and fully applicable to BWR and CANDU reactors.

The version ASTEC V2.0 will contain the main following new models and capabilities, keeping the same coupling approach CESAR-ICARE2 than CESAR-DIVA in ASTEC V1 for RCS and vessel thermal-hydraulics:

- CESAR: account for any number of non-condensable gases.
- ICARE2: all core degradation models, with mainly magma-debris formation and 2D relocation, except the detailed corium pool behaviour in lower plenum with a 2D meshing,
- ELSA: improvements of models for semi-volatile FP release (Eu, Sr, La, Ce, Ba), for UO_2 oxidation by air and reduction by hydrogen, and for SIC release,
- SOPHAEROS: preliminary model of kinetics of chemical reactions involving iodine in gaseous phase; aerosol retention in the flooded secondary side of SG.
- MEDICIS: EPR core-catcher; radiative heat transfer toward the lateral upper cavity walls and toward the vessel lower head walls; detailed thermal behaviour of these cavity concrete walls, including their melt-through; FP and concrete aerosol release.
- CPA: fast-running model for pressure suppression systems in e.g. BWR.
- IODE: sump pH computation, extension of CPA-IODE coupling in order for CPA to manage the behaviour of a iodine oxide aerosol already managed by IODE.
- New DOSE module, for computation of the dose rate in the containment gaseous phase.
- Users’ tools: coupling to a preliminary version of the JADE pre-processing tool and to the ATLAS tool for post-processing; coupling to the IRSN uncertainty analysis tool SUNSET; coupling to the IRSN probabilistic tool KANT.
- Documentation: complete and updated description of ICARE2 and CPA modules.

F. LINKS WITH OTHER SARNET TOPICS

Work has continued in the SARNET Topics Corium, Containment and Source term to converge on proposals of new modelling (or sometimes only improvements) that could be implemented into ASTEC.

Most of them come from the Source Term topic, for instance:

- SIC release from control rod [11],
- Ru release from core and behaviour in containment [12],
- Iodine radiolytic oxidation in sump [13],
- Iodine mass transfer between containment sump and gas phases [14],

In the Corium field, several activities are closely linked with ASTEC evolution:

- LIVE experiments (FZK) intensively used for validation of ASTEC models of corium behaviour and ex-vessel cooling,

- BECARRE (IRSN) and BOX (FZK) experiments and discussion on models of clad air oxidation and B_4C effects,
- Benchmarks on OLHF and FOREVER experiments for the lower head failure models,
- Discussion on the MCCI different models and validation on the international experiments, including benchmarks with other codes. This field includes phenomena such as melt spreading where different models were investigated.
- Discussion on debris coolability, in close relation with model validation on various experiments (DEBRIS in IKE, POMECO in KTH, PEARL in IRSN),
- Derivation of the material properties used in ASTEC/MDB (directly or indirectly) from the work on the NUCLEA databank.

In the PSA2 Topic, general requirements for the use of integral codes in PSA2 are being issued [15] and will be used for evaluating ASTEC. Besides, the feasibility of ASTEC coupling with dynamic PSA2 tools is being investigated.

In the Containment field, most of the time only CFD codes are used. But all benchmarks done with CFD and Lumped-Parameter (LP) codes should yield some feedback on ASTEC as recommendations to the users.

G. CONCLUSIONS

During 4,5 years in SARNET, a very large work has been done to assess the European severe accident integral code ASTEC V1. The validation was extended to many experiments, well mastered by the partners, in particular VVER-specific ones, and to several OECD ISPs. Most results can be considered as good except for core reflooding, like most existing codes, and maybe DCH. For other phenomena, such as MCCI, the models have reached the limits of the present international knowledge. Benchmarks on plant applications showed the code capability to simulate complete sequences in PWR and VVER, up to the iodine behaviour in containment and release in the environment. The general trends of results are similar between the different integral codes but some differences on results appear due to remaining differences on models, in particular on core degradation and FP transport. But it must be kept in mind that the objective of these codes is to catch the main trends and the orders of magnitude of phenomena. The comparison with the mechanistic codes on the RCS thermal-hydraulics and the core degradation give good results.

The current preparation by IRSN-GRS of the new series of versions V2 accounts for the feedback of the work performed up to now by partners and for their requirements on code evolution. The 1st version V2.0, to be released in March 2009, will include the advanced models of the ICARE2 IRSN mechanistic core degradation code (thus taking full benefit of the very intensive validation work done on ICARE2 since more than 15 years), will be applicable to EPR and will model the behaviour of Ruthenium species released after air and gas ingress into the vessel following its failure. Key areas for model improvements have already been identified for the next versions, in full consistency with the SARP WP conclusions: degraded core reflooding and in-vessel corium coolability; long-term corium coolability during molten-corium-concrete interaction; kinetics of iodine chemistry in the circuits; effect of high burn-up and MOX fuel on core degradation and FP release.

Associated with the aim to extend the ASTEC models to all European-type reactors, i.e. BWR and CANDU, the work foreseen in SARNET2 on further code assessment and providing physical models for integration into ASTEC will allow to reinforce the code as European reference for all safety studies.

ABBREVIATIONS

BU	Burn-Up of the fuel
BWR	Boiling Water Reactors
CFD	Computational Fluid Dynamics
DCH	Direct Containment Heating
EPR	European (or Evolutionary) Pressurised Reactor
FP	Fission Products
ISP	OECD International Standard Problem
ISTC	International Science and Technology Centre

ISTP	International Source Term Program
LBLOCA	Large Break Loss of Coolant Accidents
LES	Large Eddy Simulation
LOFW	Loss Of Steam Generator Feedwater Accidents
MBLOCA	Medium Break Loss of Coolant Accident
MCCI	Molten-Corium-Concrete-Interaction
MDB	Material Data Bank
MOX	Mixed Oxide fuel
PSA2	Probabilistic Safety Assessment level 2
PWR	Pressurised Water Reactors
RCS	Reactor Coolant System
RPV	Reactor Pressure Vessel
SBLOCA	Small Break Loss of Coolant Accidents
SBO	Station Black-Out scenario
SGTR	Steam Generator Tube Rupture
SIC	Silver-Indium-Cadmium alloy
VVER	Vodo Vodjannyj Energetitcheskij Reaktor: Russian acronym for Water-cooled Water-Moderated Power Reactor

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