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Overview of the integral code ASTEC V2.0

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P. Chatelard, N. Reinke

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RESUME

Ce document présente de manière générale la version V2.0 du code intégral ASTEC, co-développé par IRSN et GRS pour l'évaluation du terme source au cours des accidents graves dans les réacteurs à eau légère ou à eau lourde.

ABSTRACT

This document presents an overview of the version V2.0 of the integral code ASTEC, jointly developed by IRSN and GRS for source term evaluation during severe accidents in water-cooled reactors.

KURZFASSUNG

Dieses Dokument beschreibt die Version V2.0 des Integralcodes ASTEC, der gemeinsam von IRSN und GRS entwickelt wird zur Ermittlung des Quellterms bei schweren Unfällen in Leichtwasserreaktoren.

HISTORIQUE DES MODIFICATIONS/*CHANGE HISTORY*

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1 INTRODUCTION

This document presents an overview of the version V2.0 of the IRSN-GRS integral source term code ASTEC (Accident Source Term Evaluation Code) for severe accidents in Water-Cooled Reactors.

The aim of the code is to simulate an entire severe accident sequence from the initiating event through to release of radioactive elements out of the containment. The applications are:

- Source term determination studies,
- Probabilistic Safety Assessment level 2 (PSA-2) studies,
- Accident management studies,
- Physical analyses of experiments to improve the understanding of the phenomenology.

The code has the following requirements: sufficient validation to cover the main physical phenomena; account for safety systems and procedures; user-friendly to easily perform sensitivity analyses; equipped with tools for pre-processing, on-line visualisation, and post-processing; fast running code.

The ASTEC V1 series was developed since 1998. The latest version V1.3-rev2 was released in December 2007 to European partners in the frame of the Severe Accident Research Network of excellence (SARNET) that lasted four years (from April 2004 up to October 2008) in the frame of the FP6 (6^{th} Framework Programme) of the European Commission [ref-1]. As a continuity to SARNET, the SARNET2 project (2^{nd} phase of the SARNET network) started in April 2009 for a 4-year duration in the frame of the FP7 of the European Commission [ref-2].

While ASTEC V1 played a central role in SARNET, thus progressively becoming the reference European integral severe accident code, IRSN and GRS launched in parallel, since 2007, the development of the ASTEC V2 series. As ASTEC V1 in SARNET, the ASTEC V2 series shall continue playing a central role in SARNET2, thus confirming its status of reference European integral source term code.

The version V2.0 is being released in June 2009. As concerns the physical modelling, the two major evolutions with respect to the V1.3-rev2 version are, on the one hand, the replacement of the DIVA module by the ICARE module (directly issued from the mechanistic ICARE2 code) to deal with the in-vessel core degradation and, on the other hand, a significant evolution of the MEDICIS capabilities to allow the applicability of ASTEC V2 to the Gen-III EPR reactors, in particular thanks to a dedicated core catcher modelling. Besides these two major evolutions, most of the other physical modules (CESAR, CPA, IODE, …) have been also improved. Finally, as concerns the user tools to analyse and interpret code results, the ASTEC V2.0 version is including additional couplings to the JADE, ATLAS and SUNSET tools, respectively for pre-processing (and on-line visualisation), post-processing and uncertainty analyses.

2 REFERENCE DOCUMENTS FOR ASTEC DEVELOPMENT

The main reference documents for this ASTEC V2.0 version are:

- The general requirements of the ASTEC V2 series [ref-3],
- The general specifications of the ASTEC V2 series [ref-4],
- The general specifications for adaptation of ASTEC to different types of reactors [ref-5].

The global design choices that are described in the above general specifications are still valid (general architecture, programming language…).

Looking first exclusively at the new models which were foreseen to be issued in the first version of the V2 series, most of the specifications as described in [ref-4] have been fulfilled with the version V2.0. So, the main V2 missing physical models (which are still only planned to be implemented later, either in V2.1 or in V2.2) concern:

- Adaptation to BWRs and CANDUs of the thermalhydraulics and core degradation modelling,
- Reflooding of a severely damaged core,

- Mechanical behaviour of RCS (Reactor Cooling System) pipes and structures (i.e. induced failures).

In addition, the new CESAR/ICARE coupling (generalised coupling between the primary circuit thermalhydraulics and core degradation modules all along the whole transient) being not yet available (it is only planned for V2.1), it will be not possible in ASTEC V2.0 to properly account after lower head rupture for air ingress from cavity into the vessel (no coupling of the ICARE air oxidation model to the current CESAR thermalhydraulics).

3 MAIN EVOLUTIONS WITH RESPECT TO ASTEC V1.3-rev2 VERSION

The latest ASTEC V1 version (namely the V1.3-rev2 version) was released by IRSN and GRS in December 2007. This version was in particular extensively used in 2008 by European partners in the frame of the SARNET project and by IRSN in the frame of the PSA-2 on French PWR 1300 MWe reactors as well as by GRS within their PSA consolidation study on German KONVOI 1300 MWe PWR. This version allowed complete calculations up to iodine behaviour in containment of different sequences on PWR-900, PWR-1300, KONVOI-1300, VVER-1000 and VVER-440 operating at full power. Many applications have been performed on various accident sequences (Station Black-Out, Loss of Steam Generator Feed-Water, Steam Generator Tube Rupture, as well as Small, Medium and Large Break Loss of Coolant Accidents).

Focusing on its general capabilities, the main progress of ASTEC V2.0 compared to ASTEC V1.3 is its ability to extend the safety analyses to EPR (thanks in particular to an adequate ex-vessel modelling), its ability to investigate new designs with In-Vessel melt Retention (IVR) by external cooling, as well as the possibility to cover now the simulation of accidents in reactor shutdown states.

With respect to this previous V1.3-rev2 released version, the new ASTEC V2.0 version presents the following main model improvements:

- Extension of the CESAR module (primary and secondary circuit thermalhydraulics) to the transport of any number of non-condensable gases, as well as to pure non-condensable flows,
- New ICARE module issued from the merging of the DIVA module with the mechanistic ICARE2 code to deal with the in-vessel degradation; this major evolution provides in particular a significant improvement of the late phase models (2-D magma flows), as well as adequate models to deal with the mechanical and chemical behaviour of VVER claddings,
- Improvement, in the ELSA module, of the models of volatile and semi-volatile Fission Product (FP) release, new modelling of Ruthenium release and new model for the Silver-Indium-Cadmium (SIC) release from magmas,
- Implementation in the SOPHAEROS module of a preliminary model for kinetics of gas chemistry and of a pool scrubbing model on steam generator flooded secondary side in case of steam generator tube rupture (SGTR) accidents,
- Implementation in CPA of a new burning model to deal with the gas combustion in the containment,
- Extension of the ISODOP application to deal with several-zones in the containment,
- Implementation in the IODE module of a dedicated modelling for Ruthenium chemistry in the containment, for decomposition of iodine oxides into organic iodides and calculation of the pH value in the sump,
- Implementation of a new DOSE module to evaluate the dose rate in the containment gaseous phase,
- Significant extension of the MEDICIS module in order to be fully applicable to the EPR design; this major evolution allows in particular to manage successive MCCIs (in the cavity and in the spreading chamber), to deal with the corium slump from the cavity to the core catcher area and to evaluate the melt spreading process thanks to a simple analytical model.

In addition, as concerns especially the coupling between the different ASTEC physical modules, the main V2.0 improvements are:

- Preliminary CESAR/ICARE coupling for simulating vessel external cooling,
- Consolidation of the possibility to follow-up the in-vessel degradation calculations after the

lower head failure in order to continuously feed the MEDICIS module with slumping corium,

- Extension of the CPA/MEDICIS coupling to account for radiative heat transfers toward the lateral upper cavity walls in presence of a gaseous medium (gas being either transparent or fully absorbent or partially absorbent) and to account in the CPA zones for the gaseous sources issued from the MCCI process,
- Extension of the CPA/IODE coupling in order for the CPA module to manage the behaviour of iodine oxide aerosols as it was already done in the IODE module.

Finally, independently from the evolution of SIGAL to ODESSA, new couplings to users' tools are now available in ASTEC V2.0:

- Coupling to the IRSN JADE tool for pre-processing and on-line visualisation,
- Coupling to the GRS ATLAS tool for post-processing,
- Coupling to the IRSN SUNSET tool for uncertainty and sensitivity analyses.

4 DESCRIPTION OF THE ASTEC V2.0 MODELS

The Figure 1 in Appendix 2 presents the list of modules of ASTEC V2.0 version. It provides also an overview of the general code structure and running mode.

4.1 CESAR

4.1.1 Main modelling features

The CESAR module simulates the thermalhydraulics [ref-6] in the primary circuit, secondary circuit and in the reactor vessel (with a simplified core modelling) up to the beginning of core degradation phase, i.e. roughly up to the start of core uncovery, and in any case before the start of Zry cladding oxidation by steam. After the onset of the core degradation phase, the CESAR module computes only the thermalhydraulics in primary and secondary circuit as well as in the vessel upper plenum. The thermalhydraulics in the reactor vessel during core degradation is performed by the ICARE module.

The CESAR thermalhydraulics modelling is based on a 1-D 2-fluid 5-equation approach. Up to 5 non-condensable gases (Hydrogen, Helium, Nitrogen, Argon, Oxygen) are available. As a result 5+N differential equations and 1 algebraic equation are solved: 2+N mass differential balance equations, one for the vapor phase, N for the non-condensable gases and one for the liquid phase, 2 energy differential balance equations, one for the gas mixture phase and one for the liquid phase, 1 mixture (liquid and gas phases) differential momentum balance equation, 1 algebraic equation which models the interfacial drag between the liquid phase and the gas phase.

The interfacial drag is a complex model which has been assessed on a large number of experimental data. The break critical flow rate is based on the Gros D'Aillon correlation whereas the heat transfer coefficient between the structure and the fluid is based on a boiling curve. The different heat transfer processes are modelled: forced convection to liquid, nucleate boiling, critical heat flux, transition boiling, film boiling, forced convection to vapor and radiative heat transfer. Moreover a droplet projection model is implemented which enables CESAR to simulate core reflooding. The primary pump description is done through a 0-D approach.

The numerical method follows the finite volume technique. The space is discretized using a staggered grid with the use of the donor cell principle. The time integration is performed using a Newton's method and a fully implicit scheme is used. The Jacobian matrix inversion is based on a highly optimized Lower Upper (LU) algorithm which makes CESAR a fast running module.

4.1.2 Main V2.0 evolutions

Compared with the V1.3-rev2 version, the new CESAR models or main model improvements in V2.0 concern:

- Extension to the transport of N non-condensable gases: this new feature allows to properly manage the situations of total oxygen starvation that may occur during a reactor accidental scenario as well as to apply CESAR to circuits with any gas (either experiments or Gen.IV reactors),
- Use of temperatures T_{liq} and T_{gas} as main unknowns (instead of enthalpies H_{liq} and H_{gas}),

- Modification of a wall description: now a wall has two surface temperatures which are the main unknowns of the system (no more need for the wall temperature elimination step),
- Improvement of the interfacial fluxes (better agreement with the CATHARE laws),
- Improvement of the wall friction model (particularly for the gas phase),
- New model for liquid stratification in horizontal volumes,
- Operation in reactor states at low pressure, e.g. shutdown states or mid-loop states, keeping however in mind that the necessary validation of this new capability is not yet done (this validation should be done end-2009 at IRSN by comparison with available results of the French thermalhydraulics reference code CATHARE2).

In addition, to simplify a little bit the ASTEC input deck for plant applications, some "CONNECTI" connections which were linked to a system exclusively used by CESAR ("ACCUMULA", "PRESSURI" and "MOMENTUM") have been suppressed. The corresponding data are now directly provided within the "PRIMARY" part of the whole ASTEC input deck instead of being supplied through several separate "CONNECTI" data.

4.2 ICARE

4.2.1 Main modelling features

The ICARE module describes the in-vessel degradation phenomena (both early and late degradation phases). In the core region, the ICARE module is directly derived from the IRSN mechanistic code ICARE2 for core degradation, except for the fluid dynamics (remind that, in parallel to ASTEC runs, best-estimate safety analyses are also performed at IRSN using the ICARE/CATHARE V2 code [ref-7] which consists in a coupling of this ICARE2 mechanistic code to the French CATHARE2 two-phase thermalhydraulics reference code). In the lower head region, the physical modelling is mainly issued (along with several improvements) from the simplified DIVA modelling which was available in ASTEC V1.3 [ref-8], though also partly derived from the ICARE2 mechanistic code.

The core degradation process is characterised by the high complexity of phenomena and geometry, with a permanent appearance and disappearance of a large number of components in each control volume by melting, failure, relocation, chemical reactions, etc… This needs a dynamic management of these components. Besides, the geometry of a degraded core is very complex and heterogeneous: rod bundles with spacer grids, fluid channels blocked with molten/frozen mixtures, corium molten pool with crusts, debris beds, peripheral and lower/upper core structures (horizontal plates, vertical surrounding walls such as barrels or shrouds...), also partly or totally molten. The core is discretised in cylindrical rings and axial meshes, only one representative component of the fuel and control rods being considered in each ring, weighted by the true number of rods.

In accordance, ICARE allows to simulate the early-phase of core degradation with fuel rod heat-up, ballooning and burst, clad oxidation, fuel rod embrittlement or melting, molten mixture candling and relocation, etc… and then the late-phase of core degradation with corium accumulation within the core channels and formation of blockages, corium slump into the lower head and corium behaviour in the lower head until vessel failure. These models (both the models which are common to ICARE/CATHARE V2 and ASTEC V2 and the physical models that were specifically developed for the ASTEC lower head) are described in the ICARE2 documentation [ref-9] [ref-10].

The main ICARE2 models which can be activated in the frame of ASTEC V2.0 applications are:

- Heat transfers: axial and radial conduction between two walls, gap exchanges between rod and clad, convection between fluid and wall as well as radiation in a reactor core or in an experimental bundle whatever the degradation level is (intact rods, severely damaged core, large cavities, …). Radiation from the lower core structures to the residual water in lower plenum is also modelled, which favours vaporisation of water,
- Power: either nuclear power generated by FPs or generated in a given material, or electric power generated in some out-of-pile experiments,
- Chemistry: oxidation of Zr by steam, oxidation of stainless steel by steam, dissolution of UO_2 by solid and liquid Zr, dissolution of Zr by liquid Silver-Indium-Cadmium alloy, dissolution of Zr by solid steel, oxidation and degradation of B_4C control rods, oxidation/dissolution of relocating and relocated U-O-Zr magmas, oxidation of solid debris particles, …
- Rod mechanics: ballooning, creep and burst of Zircaloy claddings, creep of stainless steel

claddings, loss of integrity of fuel rods (using user-criteria),

- Reflooding of quasi-intact or slightly degraded cores (i.e. still in rod-like geometry),
- Material melting and relocation (both early-phase and late phase of core degradation): formation of solid debris and/or solid/liquid magma, 2D movement of magmas (axial candling of a mixture of molten and solid masses as a film along the rods or radial spreading in case of downwards obstacles), vertical collapse of solid debris, formation and expansion of a molten pool, … and then slump into the lower plenum,
- Corium jet fragmentation on contact with the water located in the lower head,
- Vessel lower head rupture: melt-through, or mechanical failure (either instantaneous plastic rupture or creep rupture) accounting for the corium and water loading on the lower head wall or user-criteria (such as temperature, degradation rate, stress).

In addition to these “standard” ICARE2 models (“standard” means “transferred from ICARE/CATHARE V2”), few specific models were specifically developed in ASTEC to avoid too high computation times:

- For core thermalhydraulics: multi-1D channel liquid and 2D gas,
- For corium behaviour in lower plenum: 2D meshing of the lower head vessel wall, combined with a 0-D approach within the plenum volume accounting for 3 stratified liquid corium layers (light metallic layer, oxide pool, heavy metallic layer) and possible debris layers.

The flexible description of geometry of vessel lower head allows simulating any type of shape such as hemispheric one for PWRs and ellipsoidal one for most of VVERs. Indeed, two alternative models are available for the vessel lower head mechanical failure though a user input option (one advised for hemispherical shape and the other one valid for elliptical shape).

On a numerical aspect, the oxidation reactions are implicited in order to properly manage the calculation of hydrogen production while reducing CPU time.

4.2.2 Main V2.0 evolutions

Compared with the V1.3-rev2 version, the replacement of the DIVA module by the mechanistic ICARE2 code to deal with the in-vessel core degradation led in particular to significant evolutions of the late phase models (2-D magma flows, oxidation/dissolution of U-O-Zr magmas, molten pool formation and expansion, …). Moreover, besides this major evolution, the ASTEC V2.0 version benefits also of several other ICARE improvements in the core region as well as of several improvements of the lower head models which already existed in DIVA. These recent model developments in V2.0 concern:

- Adequate models to deal with the mechanical and chemical behaviour of VVER claddings (dedicated model to evaluate the creep and oxidation of Zr1%Nb alloys [ref-11]),
- New general in-core heat transfer model (based on an equivalent radiative conductivity approach) able to deal with radiative exchanges in a reactor core whatever the degradation level is (intact rods, moderately degraded rods, severely damaged core, …), thus managing in a continuous way the radiative exchanges all along the evolution of the core geometry degradation,
- Possibility to define hollow structures in the lower head,
- Model to deal with the fragmentation of the hot corium slumping from the core into the water located in the lower head,
- New phase separation model (separation between metallic phases and non-miscible oxides) to be used in case of formation of a U-Zr-O-Fe molten pool in the lower head; the mass transport between the layers is calculated by assuming a quasi—steady relative motion of metal in the oxide and oxide in the metal,
- New model to manage the possible inversion of metal/oxide layers in the lower head in case the heaviest layer is above the lightest one (based on the outcomes of the MASCA experiments in Kurchatov Institute); a progressive inversion of the layers can be therefore calculated from Rayleigh-Taylor instability mechanism,
- Account for the vessel wall melting in the lower head mechanical failure model.

Moreover, to overcome some well-known V1.3 limitations (remind that, up to the V1.3-rev1 version, DIVA was automatically stopped after the vessel lower head failure), a new feature was introduced in the V1.3-rev2 version by the end of 2007 in order to possibly continue the ICARE calculations after the vessel rupture and, thus, to continuously feed the cavity pit with additional corium masses to be then used by the MEDICIS module; however, in V1.3-rev2, this new feature could unfortunately not be used as often as expected due to a lack of robustness. In accordance, efforts in that field were paid at IRSN when preparing the new V2.0 version in order to make more reliable the extension of the CESAR and ICARE calculations after the vessel rupture occurrence.

Finally, it has to be stressed that the new possibility to use a "generic" data approach (special ICARE2 pre-processing feature originally developed for ICARE/CATHARE V2 [ref-9]) should make more easy the elaboration of the ICARE part of a complete ASTEC V2 dataset for plant applications.

4.2.3 V2.0 limitations

In the current ASTEC version, it is recommended, for best-estimate plant applications, to only use the MAGMA components for representing in-core material relocation during both early and late degradation phases (MAGMA components allow to simulate both 1D candling movement of mixtures along standing rods or 2D spreading within the core in case of downwards obstacle, as well as molten pool formation and expansion in the core up to a possible pouring into the lower head). Indeed, though the DEBRIS components are already implemented in ASTEC V2.0 (DEBRIS components represent solid debris particles), they are considered as not yet enough tested to be used in a reliable way for long and complex plant applications; in accordance, waiting for an improvement of the solid debris modelling (such a task is currently underway at IRSN in the frame of the ICARE/CATHARE V2 development), DEBRIS components shall be for the moment reserved to dedicated ASTEC V2.0 simulation of late phase experiments, such as Phébus-FPT4, ACRR-MP1, …

Finally, as concerns situations or air ingress, though a dedicated air-oxidation model is available yet in the ICARE2 code (already used for ICARE/CATHARE V2 applications), these air flow conditions cannot be investigated using ASTEC V2.0 due to a lack of dedicated coupling with the ASTEC in-core thermalhydraulics (ICARE module) during the core degradation phase (this coupling is planned to be completed in the next ASTEC version).

4.3 ELSA

4.3.1 Main modelling features

The ELSA module [ref-12] [ref-13] aims at simulating the release of fission products and structural materials from the degraded core during a severe reactor accident. ELSA is tightly coupled with the ICARE module which treats the phenomena of the core degradation.

The ELSA modelling allows to describe the release from fuel rods and control rods, followed by the release from debris beds (if any) and, then, the release from the in-core molten pool. The modelling is based on a semi-empirical approach and the physical phenomena taken into account are the main limiting phenomena which govern the release.

For intact fuel rods and debris beds, the release of fission products is described according to the degree of fission product volatility. Three categories are also distinguished with the following characteristics:

<u>Volatiles</u> (such as I or Cs):

- Release is described by species intra-granular diffusion through UO_2 fuel grains, taking account of fuel oxidation (UO_{2+x}) and of a grain-size distribution,
- Te, Se and Sb can be partially trapped in the cladding depending on temperature and on the degree of cladding oxidation,
- At fuel melting point, all the remaining species located in the liquid part of the fuel are supposed to be instantaneously released.

<u>Semi-volatiles</u> (such as Ba or Mo):

- Release is described by evaporation and mass transfer processes.

<u>Low volatiles</u> (such as U or Pd):

- Release is described by fuel volatilisation treated as the vaporisation of UO_3.

The difference between the configuration of fuel rod and debris bed is the determination of the average geometrical ratio 'Surface/Volume' used in the calculation of the stoechiometry deviation.

Concerning the molten pool configuration, given the high-temperature conditions, the chemical equilibrium can be assumed in the magma so that release is governed by mass-transfer and evaporation processes from the free surface of the molten pool. Central to the modelling is the calculation of the vapour pressures of the elements in the molten pool. The assumption of a non-ideal solution chemistry is also used.

For the structural materials, release of Ag, In, Cd, Sn, Fe, Ni and Cr is taken into account in ELSA as follows:

- Ag, In and Cd (SIC) are released from degraded control rods. The same approach as semi-volatile species is used that is to say the release is described by evaporation and mass transfer processes. The SIC release happens at the control rod failure. It is followed by the release from free surface of the control rod and from the control rod molten alloys during the candling,
- Fe, Ni, and Cr are supposed to be released during the candling of steel materials, using the same approach as for the release of Ag, In and Cd,
- Sn is supposed to be released as a proportion of the rate of ZrO_2 formation (lessons drawn from Phébus.FP observations).

These structural materials can also be released from the corium molten pool.

4.3.2 Main V2.0 evolutions

The main recent developments implemented in ELSA concern the following aspects of the modelling:

Volatiles elements:

- Implementation of a new model for describing the evolution of the stoechiometric deviation. In particular, this model is used when the fuel surrounding atmosphere is air or reducing,
- Implementation of a new correlation for the oxygen partial pressure in the fuel,
- Fitting of the diffusion coefficient expression as a result of the ELSA validation carried out on the VERCORS tests, Canadian HCE3 and MCE1 test series.

Semi-volatiles elements:

- Implementation of news correlations for the partial pressures,
- New modelling for the Ruthenium release,
- Fitting of the correction factor applied to the mass transfer coefficient and the surface exchange as a result of the ELSA validation carried out on the VERCORS tests, Canadian HCE3 and MCE1 test series.

Ag, In, Cd from control rods:

- Implementation of new activity coefficients in the partial pressure expressions,
- Slight improvement of the structural materials release: corrections for the liquid fractions and better account of the free surface,
- Implementation of the MAGMA allowing to deal with Ag, In, Cd release when the 2-D general model for the corium movement is activated in ICARE.

Molten pool:

- Set a default list of atoms and species which can be considered in the model managing the FP release from a corium molten pool located inside the vessel (to prevent any conflict with the new model dealing with the FP release during MCCI (see §4.7).

4.4 SOPHAEROS

4.4.1 Main modelling features

The SOPHAEROS module [ref-14] [ref-15] simulates transport of FP vapours and aerosols in the RCS through gas flow to the containment.

Using twelve families of species (elements, compounds, gas, volatile, non-volatile…) and five states (suspended vapours, suspended aerosols, vapour condensed on walls, deposited aerosols, sorbed vapours), the mechanistic and semi-empirical approaches model the main vapour-phase and aerosol phenomena:

a/ Vapour-phase phenomena

- Gas equilibrium chemistry. The reference databank (in MDB) contains about 800 species,
- Chemisorption of vapours on walls,

- Homogeneous and heterogeneous nucleation,
- Condensation/revaporisation on/from aerosols and walls,
- Preliminary model for kinetics of gas chemistry.

b/ Aerosol phenomena

- Agglomeration: gravitational, Brownian diffusion, turbulent diffusion,
- Deposition mechanisms: Brownian diffusion, turbulent diffusion, eddy impaction, sedimentation, thermophoresis, diffusiorophesis, impaction in bends. Deposit of aerosols in a flow contraction (either abrupt one with a 90° angle or conical) can be simulated,
- Remobilization of deposits: revaporisation and mechanical resuspension. Two models are available for aerosol mechanical resuspension: the "Force balance" model and the “rock and roll” one (based on the JRC approach),
- Dedicated pool scrubbing model for steam generator flooded secondary side.

Materials for primary circuits of CANDU reactors have been implemented along with the corresponding chemisorption correlations.

4.4.2 Main V2.0 evolutions

Compared with the V1.3-rev2 version, the recent SOPHAEROS improvements in ASTEC V2.0 focused on:

- Implementation of a preliminary model of kinetics of chemical reactions in gaseous phase (focusing first on the Cs-I-O-H system), validated on Phébus FPT1 (validation is being now continued against the IRSN CHIP experiments),
- New pool scrubbing model to deal with the retention of aerosols in the secondary side of flooded steam generators (in case of SGTR scenario), validated on PSI ARTIST experiments.

4.5 RUPUICUV

The RUPUICUV module [ref-16] simulates the DCH (Direct Containment Heating), i.e. ex-vessel discharge of hot corium into the cavity after lower head failure (vessel blow-down, cavity pressurisation) and potential corium oxidation and entrainment from the cavity to the containment.

Two kinds of cavity geometry are considered:

- “Closed” cavities such as in USA-type PWRs, i.e. without direct connexion with containment, but through a series of intermediate compartments,
- “Open” cavities such as in Western European PWRs, i.e. with an annular space around the vessel towards the containment.

A simplified model describes the entrainment kinetics, with the assumption of instantaneous suspension of corium in cavity. Droplets entrainment by the gas flow is the predominant mechanism for corium entrainment from cavity into the containment. The entrainment efficiency is evaluated from the ratio of the relative velocities particle/gas in the annular space (based on gas/particle friction depending on particle size). A simplified particle flow path in the cavity is assumed.

The particle size is either given by the user or calculated with the Weber number. Particle trapping in compartments between cavity and containment is directly taken into account through the global correlation of entrained corium. In the case of "open" geometry, this global correlation was fitted on analytical Surtsey and KAERI experiments that were performed in this geometry.

Heat transfer debris/gas is assumed instantaneous in cavity (complete gas/debris thermal equilibrium). Oxidation of the entrained corium (zirconium and steel) is modelled without any reaction kinetics.

The user can activate the DCH module while representing the cavity as a CPA volume: this representation is recommended for a better coupling MEDICIS-CPA (see §5.2).

No model evolution was performed with respect to ASTEC V1.3-rev2.

4.6 CORIUM

This simple parametric module [ref-17] simulates the behaviour of corium droplets transported by HPME (High Pressure Melt Ejection) into the containment atmosphere and sump. Hot gases entrain these droplets. Heat transfer between corium and gas is modelled in each containment zone (DCH).

Major uncertainties concern the particle path and flight time.

No model evolution was performed in ASTEC V2.0 with respect to the V1.3-rev2 version.

4.7 MEDICIS

4.7.1 Main modelling features

The MEDICIS module [ref-18] simulates MCCI (Molten-Core-Concrete Interaction) using a lumped-parameter 0-D approach with averaged melt/crust layers. Corium remaining in the cavity interacts with concrete walls. This module assumes either a well-mixed oxide/metal pool configuration or a possible pool stratification into separate oxide and metal layers. It describes concrete ablation, corium oxidation and release of incondensable gases (H_2, CO, CO_2) into the containment. Most convective heat transfer correlations available in literature for the corium/concrete interface (Kutateladze, Bali, …) and the interface between corium layers (Greene) are implemented.

Its structure is flexible enough to allow an easy implementation of new models generated by R&D outcomes. A robust algorithm for cavity erosion was developed, including the possibility to represent a multi-layered concrete basemat. The module is interfaced with the general physico-chemistry package MDB (see §4.14) for element speciation in a mixture, thermodynamic data (liquidus and solidus temperatures, mass and volumetric solid fractions…), and thermo-physical properties (density, viscosity…).

The MEDICIS module contains:

- A model of the structure of the corium/concrete interface taking into account from the pool bulk to the concrete interface a convective zone, a conductive zone described as a mushy crust and a slag layer similar to that of CORCON code ; the boundary temperature between pool convective and conductive zones, called solidification temperature, is a crucial parameter ; the intensive validation led to recommend a temperature lower but close to the liquidus one ;
- Models of corium coolability in case of water injection upon the corium pool surface (derived from models from the US/NRC CORQUENCH code), including water ingression through the upper crust and corium eruption through the upper crust towards the overlying water pool ;
- Models of evolution of corium pool configurations, depending on criteria using the superficial gas velocity and the difference between layer densities determining the switch between homogeneous and stratified pools ;
- Capability to account for successive MCCIs (useful feature to simulate MCCI in the EPR cavity and then in the spreading chamber), keeping in mind that, in V2.0, only sequential MCCI in different volumes is possible up to now (that means MCCI in the first volume stops when MCCI in the second one starts) ;
- Corium pouring kinetics from the cavity towards the core-catcher (EPR design) using a simple model (based on a combined use of a Bernoulli flow approach and of properties from MDB) ;
- Models to evaluate the release from the ex-vessel corium pool of concrete aerosols and the release of fission products during MCCI ;
- Use of the MDB package to evaluate the corium layers properties.

A tight coupling between MEDICIS and CPA modules through a prediction-correction method is possible (see §5.2).

4.7.2 Main V2.0 evolutions

Most of the recent improvements are directly linked to the special concept of EPR core catcher:

- Extension to describe MCCI in successive cavities, introduction of corium pouring from the cavity pit to the spreading chamber ;
- Approximate evaluation of the melt spreading capability thanks to a simple analytical model (combination of the fraction of the occupied area and of a spreading kinetics).

Compared with the V1.3-rev2 version, the few other recent improvements in ASTEC V2.0 focused on:

- Improvement of heat transfer models (in particular heat transfer description by natural and solutal convection), with a continuous validation on the ongoing experiments in real or simulant materials (VULCANO, OECD-CCI, ARTEMIS, …),

- Heating and ablation of upper cavity concrete walls ;
- Radiative heat transfers in the cavity taking into account with user's parameter absorption length the absorption by atmosphere (containing steam, carbon dioxide or concrete aerosols),
- Introduction of a corium viscosity law as a function of solid volume fraction,
- Evaluation of the FP release during MCCI (model derived from that of ELSA assuming the FP vapours are transported by gas bubbles),
- Empirical model to evaluate the aerosol production during MCCI ; this model, proposed in 1997 by A. Shubenkov (Kurchatov Institute), is based on the evaluation of the concrete aerosol concentration above the pool using an empirical approach with parameters fitted on ACE experimental data and it determines the aerosol mass release rate in proportion to the gas volumetric rate escaping out of the pool.

4.8 CPA

The CPA module [ref-19] [ref-20] simulates thermalhydraulics and aerosol behaviour in containment. It consists of two main sub-modules THY (for thermalhydraulics) and AFP (for aerosols and FPs). The containment discretisation through a "lumped-parameter" approach (0-D zones connected by junctions) simulates simple or multi-compartment containments (tunnels, pit, dome…) with possible leakages to the environment or to normal buildings, with more or less large openings to the environment.

4.8.1 Thermalhydraulics in containment

CPA-THY models are based mainly on the models of the former German containment codes: RALOC Mod4 and the thermalhydraulics part of FIPLOC. They describe phenomena such as pressure and temperature build-up and history, local temperature and pressure distributions, local gas distributions (steam and different non-condensable gases), local heat transfer to walls (free and forced convection, radiation, condensation), 1D heat conduction in structures (plate or cylinders, consisting of several material layers), and hydrogen combustion.

The thermalhydraulics state of a node can be described according to two concurrent approaches:

- Either by the equilibrium model assuming water and atmosphere homogeneously mixed for saturated and superheated (no water) conditions, that is water and gases at the same temperature,
- Or by the non-equilibrium model where deposited and airborne water are separately balanced, i.e. with their own energy (separate temperatures and mass balances for atmosphere and water sump) and mass balances.

Mass transfer between zones is described separately for gas and liquid flows by momentum equations (unsteady, incompressible or steady compressible) accounting for the height differences between zone centres.

In ASTEC, combustion occurs according different criteria: user-input or crossover of flammability limits in the Shapiro diagram. For the latter, 4 different flammability limits determined at atmospheric pressure and room temperature are defined on the ternary Shapiro diagram hydrogen-air-steam.

Independently from the COVI and PROCO modules which are discussed in a separate section (see §4.9), two different models were available in ASTEC V1.3 to simulate hydrogen combustion in CPA: a detailed one, DECOR for laminar hydrogen deflagration, and a simplified one, COMB [ref-21]. The latter uses a parametric approach and is fully coupled with CPA; it models situations where flame propagation is not an important issue. To overcome this COMB limitation, a third model, namely the CPA-FRONT model, was recently developed at GRS and is now also available in the V2.0 version (see next paragraph).

The combustion model COMB in CPA provides a volume defined, thermodynamical correct calculation of the combustion in one or several zones. As the ignition time and the burning duration is defined by the user, no propagation of the combustion from a burning zone to an non-burning zone is simulated. Therefore, the combustion model COMB in the containment module CPA has been extended by a model for the flame front propagation. This model provides ignition time and burning duration for the CPA zones. It is an alternative to the user defined or PROCO pre-calculated values. The propagation of the flame front takes place along the 1D network comprising of the junctions between the containment zones. The flame front velocity is the sum of gas velocity and combustion velocity. Therefore a correct treatment of the interaction of combustion and flow is given. The turbulent flame velocity is calculated by the Flamelet model of Peters. By integrating the flame front velocity the position of the flame front is obtained. Since there is no calculation of the turbulent intensity in the lumped parameter code, an adequate correlation has to be selected. The turbulent intensity is a function of Reynolds Number. Actually correlations from PROCO are taken.

For a realistic description of the accident, models represent the main phenomena involved in engineered safety systems such as spray systems, recombiners, and pressure suppression systems as in VVER-440 bubble condenser towers (through the DRASYS model).

Besides the detailed recombiner models, fast running correlations were added [ref-22], faster and simpler to use. Two kinds of such correlations are available for the simulation of different kinds of Siemens Passive Autocatalytic Recombiner (PAR) type FR90/1series. But they do not give any information on PAR temperature or outlet concentration, on velocity, on mass flow rate.

Main V2.0 evolutions

Compared with the V1.3-rev2 version, the main model improvements in ASTEC V2.0 on CPA thermalhydraulics concern:

- Implementation of a new burning model (so-called “CPA-FRONT” model) to deal with the gas combustion in the containment,
- Implementation of the fast running, simplified INSERTION model to simulate the submergence of vent pipes into a pool, which bases on the ATM_VALVE model (atmospheric junction equipped with a valve into the FLUID part of a NONEQUILIB zone),
- Improvement of the DRASYS condensation model (better numerical stability).

In addition, the V2.0 version fully benefits from the significant improvement of the CPA restart capabilities which was only achieved in 2008, i.e. after the delivery of the V1.3-rev2 version.

4.8.2 Aerosol and FP behaviour in containment

CPA-AFP models for aerosol transport and depletion [ref-23] are based on the FIPLOC code. They describe phenomena such as volume condensation and growth of insoluble and soluble aerosol particles, behaviour of chemically different aerosol components, and agglomeration and deposition processes. The transport model FIPHOST [ref-24] is included to calculate the decay heat of gaseous and particulate FP and their transport/depletion by the different hosts like water or walls in atmosphere or in sump.

The aerosol calculation is based on the poly-disperse MAEROS model. The aerosol retention through water pools is simulated with the pool-scrubbing model SPARC-B.

The behaviour and effect of spray systems is thoroughly modelled: effect on thermalhydraulics and on aerosols, on the basis of validation on CARAIDAS (IRSN) and CSE (USA) experiments [ref-25], wash-out of FP and aerosol deposits on the containment walls.

Main V2.0 evolutions

Compared with the V1.3-rev2 version, the main model improvements in ASTEC V2.0 on aerosol and FP behaviour concern:

- Extension of the CPA/IODE coupling in order to allow CPA managing the behaviour (transport, depletion) of iodine oxide aerosols (such a task was already managed by IODE),
- Account for the aerosols retention in the leakages in the containment walls,
- Improvement of the starting conditions for the Containment Spray System (better consideration of the tank option).

4.9 OTHER HYDROGEN COMBUSTION MODULES

The COVI module [ref-21] computes in a very simple way the maximal value of built-up pressure in adiabatic conditions of hydrogen combustion (AICC: Adiabatic Isochoric Complete Combustion). It yields the situation of the whole containment in the Shapiro diagram, and the temperature and pressure peaks at current time as if H_2 and/or CO were instantaneously burnt. The available hydrogen in all CPA compartments is summed up and burnt down to a user-defined percentage. The energy is distributed on the total volume of all compartments. There is no feedback on CPA calculations, but only an evaluation of this pressure that can be considered as a maximal envelope value. It is activated either at a time selected by the user or when one of the 4 flammability limits (see §4.8.1) is crossed in a given compartment or cell.

The recent improvements in ASTEC V2.0 focused on:

- Implementation of a “multi-domain” functionality, i.e. the extension of the P_{AICC} and T_{AICC} calculation to n domains (a domain being a cluster of CPA zones) in order, for instance, to be able to compute the virtual combustion in both the inner containment and the inter containment space for configuration like in the French PWR-1300 MWe.

An additional detailed model for H_2 combustion was implemented in a separate module besides the existing DECOR model in CPA: the PROCO module of H_2 combustion (developed by IRSN [ref-26]) simulates slow and fast turbulent deflagration processes. Its application scope is complementary from the DECOR one. Its use needs a “cubic” sub-nodalisation of the CPA zones, which takes into account the real connections in the plant to be investigated. It can be used in 2 different modes:

- Either stand-alone without any feedback of results to CPA, i.e. in a "virtual" evaluation of consequences of H_2 combustion at a given point of the scenario. In that case, CPA needs to be started first and then CPA delivers the gas distribution and concentrations at start of PROCO,
- Or with feedback to CPA, what allows continuing the scenario calculation after burning some amount of H_2 during this combustion. The total burning time of the combustion in the different PROCO zones belonging to a CPA zone is summed up and transferred to COMB together with the ignition time of PROCO. Then the combustion process is repeated by COMB model in CPA, taking into account the energy release, mass changes and the movement of the gases.

4.10 IODE

4.10.1 Main modelling features

The IODE module [ref-27] simulates iodine behaviour in the containment, focusing on the roughly twenty-five predominant chemical reactions in sump, gas phase and at contact with surfaces. More precisely, it describes in a kinetic way (i.e., non-equilibrium) the chemical transformations of iodine.

As concerns the transport of iodine species through compartments of the containment, it is computed by the CPA module.

<u>a/ Reactions in sump</u>

The main modelled phenomena are:

- Hydrolysis of molecular iodine,
- Radiolytic oxidation of I^- (Evans-Liger) in sump, where oxidation is dependent on rate production of OH radicals, and where I_2 reduction is temperature-, pH- and $[I^-]$-dependent.
- HOI dissociation/disproportionation,
- Iodide oxidation by the oxygen dissolved in the sump water,
- Formation of methyl iodide by homogeneous reaction: Taylor’s homogeneous model where solvents are released from paint in liquid phase, then oxidized under radiation to form organic acids, and finally RI are formed by interaction between I_2 and solvents or sub-products,
- Methyl iodide radiolytic decomposition,
- Silver iodide formation by heterogeneous reactions (Ag_{ox}/I^- and Ag/I_2),
- Adsorption/desorption of molecular iodine.

<u>b/ Reactions in gas phase</u>

The main modelled phenomena are:

- Kinetics of O_3 formation,
- Oxidation of molecular iodine in iodate by O_3 air radiolysis products,
- Organic iodide formation either by an homogeneous model or by the Funke heterogeneous model,
- Gas phase radiolytic destruction of organic iodine, based on work performed in the ICHEMM FP5 project, especially on AEA-T experiments,
- Mass transfer between sump and gas phase, which can now be computed instead of being

defined by user parameters, and deduced from the interpretation of IRSN SISYPHE experiments. This model is also available in evaporating conditions,

- Iodine adsorption/desorption on painted, metal and concrete walls,
- Effect of spray on molecular iodine: mass transfer between gas phase and droplet, interfacial equilibrium at the droplet surface, liquid mass transfers inside the droplet, chemical reactions in the bulk liquid. The module computes kinetics of the overall process during the droplet fall down and the output information is the rate of capture of I_2 for each compartment,
- Dedicated model of Ruthenium chemistry occurring in gas phase (specific attention was recently paid at IRSN to Ruthenium because, in severe accident conditions, gaseous Ruthenium can be formed and released outside the containment, thus inducing, at short and middle term, significant radiological consequences that have to be considered for emergency safety plan).

4.10.2 Main V2.0 evolutions

Compared with the V1.3-rev2 version, the main recent IODE improvements in ASTEC V2.0 have concerned:

- Modification of the decomposition of organic iodides in the gaseous phase,
- Account for the decomposition of iodine oxides into organic iodides,
- Implementation of a dedicated modelling for the Ruthenium behaviour in order to complete FP chemistry models inside the containment, based on IRSN EPICUR experiments,
- Addition of the calculation of the pH value in the sump.

<u>Warning</u> : As concerns the pH evaluation, the V2.0 model is not yet applicable to full scale analyses. It means that it could be applied in ASTEC V2.0 to small-scale experiments simulations but not to plant applications for which the current modelling is not yet valid.

4.11 DOSE

A new DOSE module, which was not existing in ASTEC V1.3-rev2 (it was originally developed in ASTEC to answer IRSN PSA-2 requirements), is now available in ASTEC V2.0.

The DOSE module [ref-28] allows to evaluate the dose rate in the containment gaseous phase. It has however to be underlined that, up to now, this module was only validated by comparison with dedicated IRSN codes.

4.12 ISODOP

The ISODOP module [ref-29] simulates decay of FP and actinide isotopes in different zones of the reactor.

It starts the calculation using an initial isotope inventory generated by the CEA code PEPIN and allows decay heat and activity in the core, in the RCS, in the containment and in the environment to be estimated. It is based on the DOP database from CEA containing a description of 720 isotopes.

The management of neutron and residual power in a ASTEC calculation is described in [ref-30].

Compared with the V1.3-rev2 version, recent improvements in ASTEC V2.0 have concerned the extension of the ISODOP applications to correctly deal with several-zones in the containment.

4.13 SYSINT

The SYSINT module [ref-31] allows the user to easily simulate the management of engineered safety features (for instance, safety injection systems, pressurizer spray and heaters, management of steam generators, containment spray system in direct or recirculation mode, hydrogen recombiners,…).

4.14 MDB

This library Material Data Bank (MDB) [ref-32] groups together all material properties under a unique simple readable format. This includes:

- All simple materials of a water-cooled reactor (solid, liquid and gas) and associated usual properties (enthalpy, conductivity, density…),
- Ideal chemistry (equilibrium reactions),
- Iodine chemistry in containment (kinetics),
- FP isotopes (decay heat, transmutation rates…),
- Complex materials such as molten corium.

The MDB library includes all the recent research on the nuclear material properties done in international projects: CIT and ENTHALPY FP4 projects for FP and OECD, RASPLAV and MASCA projects for corium. The evaluation of corium properties is based on the European NUCLEA database for corium thermo-chemistry [ref-33] [ref-34].

A graphic interface is provided allowing users for plotting properties, updating them if necessary, checking the modifications.

In the ASTEC V2.0 version, MDB is only used in the following modules: ELSA and SOPHAEROS for FP gas equilibrium databanks, ISODOP for isotopes evolution, IODE for iodine chemical reactions, and MEDICIS for corium properties. The extension of its use to other modules (CESAR, ICARE, RUPUICUV and CPA) is planned in the next ASTEC V2.1 version.

In ASTEC V2.0, the main improvements with respect to the MDB version delivered with ASTEC V1.3 concern the review and improvements of the properties of species related to Mo, Te and Ru in the gas chemistry databank used by SOPHAEROS module, keeping in mind that a report describing the detailed content of the MDB in ASTEC V1.3 was released in 2007 [ref-35].

The main future improvements should concern the treatment of complex materials. Two directions for getting data are studied: building tables using a code like GEMINI, or using an efficient Gibbs minimization solver directly implemented in MDB. A first version of tabulated properties is now available, with applications to the U-O-Zr and U-O-Zr-Fe diagrams. Studies are also going on to further develop better chemical equilibrium solvers.

5 CODE STRUCTURE AND OPERATING MODE

5.1 GENERAL STRUCTURE

The code structure is modular, each of its modules simulating a reactor zone or a set of physical phenomena. The code size is about 450000 instructions and more than 2000 subroutines.

The ASTEC modules communicate with each other through a “dynamic” memory. A specific tool, SIGAL, was developed in Fortran 95 for managing this database. This tool allows in particular a checking of syntax and consistency of input data, the uniqueness of data and a dynamic management of memory size. Moreover, in ASTEC V2, some new capabilities have been added to the SIGAL ones through the development of another specific tool, named ODESSA (ODESSA provides in particular an adequate frame to progress towards programming parallelisation and it allows also to manage some recursivity of the SIGAL-like procedures, that is in particular necessary to activate new 2D visualisation procedures).

Two different running modes are possible in ASTEC V2.0 (Fig.1):

- Stand-alone mode for running each ASTEC module independently, which is useful for module validation,
- Coupled mode where all (or a subset) of the ASTEC modules are run sequentially within a macro-time step. This mode allows explicit feedback between modules.

The code is developed and managed within a framework of Quality Assurance procedures: programming rules, software tool for version management and change control, and complete documentation.

The code is running on both PC-Linux and PC-Windows (NT or XP operating systems for the latter) and it requires a 1Gb RAM to operate correctly.

5.2 SPECIFIC COUPLING MODES BETWEEN MODULES

5.2.1 CESAR-ICARE coupling

During the front-end phase, CESAR alone calculates the thermalhydraulics in the whole RCS [ref-36], using a simplified core modelling of 1 radial mesh. An automatic switch to ICARE for simulation of in-vessel core degradation phenomena is then applied (see Figure 2 in Appendix 2), similarly to the one which had been elaborated for DIVA in ASTEC V1, depending on specific criteria e.g. void fraction in primary circuit loop, void in the upper plenum, void fraction at the top of the core, steam temperature at the top of the core, and non isolated accumulators mass fraction. This switch becomes effective around time of start of core uncovery, and in any case before the start of Zry cladding oxidation by steam. After the switch, CESAR calculates only the loops and the vessel upper plenum, and ICARE calculates the remaining part of the vessel (core, lower plenum and downcomer).

A specific prediction-correction coupling approach was developed in ASTEC V1 between CESAR and DIVA [ref-36]. A prediction technique was adopted in DIVA to evaluate the RCS thermalhydraulics, using the CESAR circuit as defined by the user. DIVA was using as inputs the CESAR outputs from the previous macro time step. The two numerical schemes were disconnected and each module was running at its own time-step. Meeting points occurred at the end of an intermediate macro time-step. This macro time-step management had been differentiated from the other modules in order to gain CPU time.

In ASTEC V2.0, though few improvements were applied in ICARE to try making the prediction phase more adequate (better estimation of the void fraction in the circuit for instance), the same coupling approach CESAR-ICARE than CESAR-DIVA in ASTEC V1 was kept for the thermalhydraulics in the RCS and in the vessel. It means that, though unfortunately associated to some well-known drawbacks, the switch to ICARE at the end of the front-end phase will still remain necessary in the V2.0 version. Indeed, the new coupling technique, which shall allow CESAR to cover the thermalhydraulics in the whole RCS (vessel and loops) during the whole transient (thus allowing to suppress this switch step), is only planned to be implemented in the future V2.1 version.

Anyway, compared to the previous V1.3-rev2 revision, a new CESAR-ICARE coupling functionality has been developed in ASTEC V2.0 for simulating the vessel external cooling, thus allowing to manage In-Vessel Retention conditions which are expected to occur in some VVER-440 or some Gen.III reactors (this extension of the previous CESAR/DIVA coupling was validated by CEA partner in SARNET frame [ref-37] on the SULTAN, ULPU and, in a preliminary way, LIVE experiments).

5.2.2 MEDICIS-CPA coupling

A specific prediction-correction coupling approach was developed between MEDICIS and CPA when representing the cavity as a CPA volume.

First, in the prediction step, MEDICIS calculates the whole behaviour of the cavity with some simplifications. This module computes the radiative heat exchange between the upper surface of the corium, the internal wall surfaces (of the reactor pit or lower head reactor vessel) and the gas. The gas is considered as grey and can be transparent, fully absorbent or partially absorbent. The gas flow rates coming from the MCCI are taken into account as well as heat exchanges between the upper layer and water sump (convective heat transfer computed by the water ingression model).

All these heat fluxes are then transferred to CPA which, in the correction step, calculates again the cavity thermalhydraulics in the same time as the other containment zones, taking into account the gas mass flow rates entering into this zone or going out of this zone. CPA calculates also the convective heat fluxes on the wall surfaces, which are then taken into account by MEDICIS in the following time step.

Compared to the previous V1.3-rev2 revision, the MEDICIS-CPA coupling has been improved as follows:

- Account for radiative heat transfers toward the lateral upper cavity walls and toward the vessel lower head walls (assuming a gas medium with imposed absorption properties in the cavity),
- Detailed thermal behaviour of these lateral upper cavity concrete walls, including their melt-through (the walls are no longer considered as adiabatic),
- Transfer into CPA zones of the gas sources produced during MCCI, for the consequences in the containment.

5.3 USERS' TOOLS

The computer interface, mostly based on the SIGAL-ODESSA softwares [ref-38] [ref-39], includes:

- An automatic data checker at the pre-processing step,
- Tools for processing ASTEC results, mainly described in [ref-40], consisting of on-line

visualisation tools and of the front-end Graphic User Interface processor GTIC that helps to build graphical files with the TIC tool [ref-41].

In ASTEC V2.0, new pre-processing and on-line visualisation capabilities are now available thanks to a coupling to a preliminary version of the IRSN JADE tool which includes a Graphical User Interface (GUI). JADE is especially designed to help users in elaborating ASTEC input decks as well as in making easier the checking of complex ASTEC V2 input decks.

As concerns post-processing, the coupling with the GRS ATLAS graphical tool is being progressively extended to all modules (today available for CESAR, ICARE, SOPHAEROS and CPA). It allows off-line visualization of results, either in the form of 2D colour graphics of containment or RCS, or of curves of evolution of variables in the SIGAL database along time. ATLAS (with its graphical editor APG) allows the user to set up its own plant graphics with its own nodalisation scheme for dynamic visualisation of the selected parameters. As in the V1.3-rev2 version, two pre-defined colour graphics (the first one for a KONVOI 1300 MWe PWR and the second one for a VVER-1000 MWe reactor) are available in ASTEC V2.0.

The coupling of ASTEC to the IRSN SUNSET uncertainty tool was recently achieved in order to make easier the realisation of sensitivity analyses thanks to an evaluation of the influence of uncertainties on data or models on the code results.

Finally, knowing that IRSN developed the KANT dynamic reliability tool to answer PSA-2 requirements, automatic couplings with dynamic PSA-2 methods are underway at IRSN through CPA/KANT coupled applications.

5.4 CODE MAINTENANCE

For exchange of information between users and the maintenance team, a specific tool MARCUS was set up in 2004 and a new MARCUS version is now operating (to be accessed at the "www-marcus.irsn.fr" web address). This tool assures the survey and storage of all request cards sent by users to indicate anomalies when running the code, along with the corrective action carried out by the maintenance team to overcome the problem.

6 CODE DOCUMENTATION

Many efforts focused on the improvement of the code documentation, which was the main request from code users in SARNET frame.

A first step of improvements was already reached with the V1.3 version. Indeed, in addition to the usual release guide (summarising the main differences between the V1.2 and V1.3 versions and providing the list of the V1.3 delivery test-cases along with their main results), the main updates of the ASTEC V1 documentation concerned at that time:

- More homogeneous format of description of physical models: 1 document per module (except for CPA). The pdf format allowed hyperlinks between different documents on the CD-ROM. For the first time, the description of two important couplings, CESAR-DIVA and MEDICIS-CPA, was added,
- Description of main outputs in a specific directory of the code CD-ROM,
- Description of the detailed content of the MDB library,
- First version of Users Guidelines covering the essential recommendations (this first version was not exhaustive but it was enriched progressively later on through successive updates associated to successive V1.3 revisions).

The efforts to improve the code documentation have continued since the release of the V1.3-rev2 version end-2007, so that a second step of improvements has been reached with the V2.0 version:

- In-depth review and update of the ICARE documentation (both the user's manual [ref-9] and the theoretical manual [ref-10], the latter being not yet completed),
- In-depth review and update (still in progress) of the CPA documentation [ref-19] [ref-20], including the description of the new CPA-FRONT model,
- In-depth review and update of the MEDICIS theoretical manual [ref-18],
- Update of the SOPHAEROS user's manual [ref-14],
- Update of the theoretical manuals for CESAR, SOPHAEROS and IODE modules [ref-6] [ref-15] [ref-27],

- Update (still in progress) of the theoretical manual for ELSA modules [ref-13],
- New report describing the DOSE module [ref-28],
- Corrections of the HTML on-line users manuals (this action being a recurrent one, it will of course go on after release),
- New version of the Users Guidelines [ref-42] covering the essential V2.0 recommendations (as concerns specifically the core degradation processes, the latest version of the so-called “ICARE2 users’ guidelines” [ref-43] is also bringing valuable comments and advises to be accounted for by users to elaborate ASTEC V2.0 input deck),
- Release guide, exclusively focused that time on the delivery test-cases with their main results [ref-44], keeping in mind that the main differences between the V1.3-rev2 and V2.0 models are summarised in the present document.

7 ASSESSMENT OF THE V2.0 VERSION

7.1 VALIDATION METHODOLOGY

As it was already the case for ASTEC V1, the ASTEC V2 validation will be supported by a large set of French, German and international experiments that cover most aspects of severe accident phenomenology. The main principles of validation were defined in [ref-45] and are still valid.

Two levels of validation efforts are defined:

- The basic validation matrix (see Tables 1 to 5 in Appendix 1), partly based on ISPs (International Standard Problems of OECD). A “minimum” set of about 25 experiments is recalculated again at each major code release: this allows the applications to reactor-cases to be tackled with an acceptable degree of confidence.

- The extensive matrix gathers all experiments that are calculated (or have been calculated with previous code versions) besides the minimal ones. It represents about twenty to thirty experiments per module.

The validation matrix mainly includes Separate-Effect Tests (SET) or Coupled-Effect Tests (CET) that cover most phenomena. It also includes integral applications such as the TMI-2 accident and the integral experiments of the Phébus.FP programme, particularly the application to the OECD ISP N°46 on the FPT1 experiment (this application coupled all the modules involved for the primary circuit and for the containment).

7.2 VALIDATION STATUS

As regards the physical models which were already available in previous code versions, ASTEC V2.0 fully benefits of course from the intensive validation which was carried out between 2004 and 2008 not only by GRS and IRSN but also by SARNET partners using successively the previous V1.2-rev1 and V1.3-rev2 versions [ref-46] [ref-47]. Indeed, the main conclusion of this significant ASTEC V1 validation work is the fair to good agreement with experimental data, even in some cases with an excellent agreement [ref-48].

More precisely, the circuit thermalhydraulics models, which have been assessed against various test configurations (PATRICIA GV, REBECA, SUPER-MOBY-DICK, BETHSY, PMK2, PACTEL, LOFT, TMI-2 …), have been proven to give good results, not far from the ones of mechanistic codes [ref-49].

Except for reflooding of degraded cores, the core degradation models, which have been assessed against various operating conditions (Phébus.FP, CORA and QUENCH rod-bundles, OLHF, FARO and LIVE lower heads, TMI-2, …), led also to often get good results, still not far from the ones of mechanistic codes [ref-49]. Moreover, the modelling limitation of 1-D candling relocation process of molten mixtures along the rods is cancelled in the ASTEC V2.0 version: the 2D magma relocation models (transferred from the ICARE2 code – *see §4.2*) allow now a much more realistic simulation of the in-vessel late-phase, especially as regards kinetics of corium relocation to the lower plenum, which is important for the management of the accident. More generally, as concerns the core degradation processes, the ASTEC V2.0 version also benefits from the very extensive assessment that was performed during the last ten years on the ICARE2 IRSN code [ref-50].

The MCCI models are at the state of the art but they showed yet, like all other codes, a lack of predictability. The use of a unique set of assumptions on the corium-concrete interfaces allowed performing an overall consistent interpretation of real material experiments in homogeneous oxide corium configurations for limestone-sand or siliceous concrete types in OECD-CCI and VULCANO programs [ref-51]. The next step, currently under progress at IRSN, is the interpretation of VULCANO experiments in corium stratified configurations.

As concerns FP release models, though overall good results were often obtained under various conditions (VERCORS, VI, Phébus.FP,… [ref-52]), some discrepancies remained in ASTEC V1 on release of semi-volatile FP from fuel rods and of SIC (Silver-Indium-Cadmium) materials from control rods but model improvements have been implemented in ASTEC V2.0, which should lead to significantly reduce these discrepancies.

For FP transport in RCS, good results were obtained against VERCORS HT, TUBA, STORM, COLIMA, …. [ref-52]. Nevertheless, a significant progress for speciation was the recent development in ASTEC V2.0 of a detailed gas chemistry modelling, despite it made the assessment much more complex. A preliminary assessment has been successfully achieved against the Phébus.FPT1 experimental data and the validation is now being extended to the IRSN CHIP experiments.

The DCH models validation against the ANL, SNL and DISCO experiments concluded that these models were too parametric and too geometry-dependent. Although the importance of this phenomenon is much lesser for Gen.III NPP designs, model improvements are planned in the next ASTEC V2.1 version.

Good results were obtained on the containment thermalhydraulics models [ref-52], for instance on the following experiments: ISP47 on TOSQAN, MISTRA and ThAI facilities, CARAIDAS and CSE A10 on spray [ref-53], and recently the PANDA experiments in the frame of SETH-II OECD project [ref-54].

As to iodine behaviour in containment, ASTEC V1 validation results (in particular against Phébus.FP [ref-55] and ThAI) could be considered as good despite some discrepancies due to the model of formation of organic iodides in the gaseous phase and to the lack of knowledge on iodine oxides behaviour. In ASTEC V2.0, the accuracy of these two models have been improved (see §4.10), in particular using the IRSN EPICUR experiments [ref-56], currently performed within the International Source Term Program (ISTP). The applicability of the models to multi-compartment containment configurations was proved by the validation on the ThAI experiments [ref-57].

7.3 NEXT STEPS IN THE VALIDATION PROCESS

In summary, independently from the good conclusions drawn from the extended V1.3-rev2 validation, the ASTEC V2.0 has been assessed before its delivery against more than 20 experiments ("minimum" set of experiments which is systematically recalculated at each major code release – *see §7.1*) as well as against several other experiments (separate validation of new models using each ASTEC module in a stand-alone mode). Moreover, it has to be underlined that, within the next 12 months, validation work will continue intensively using the V2.0 version in the particular frame of the SARNET phase 2 project (most of the experiments which were calculated in 2008 with the V1.3-rev2 version will be recalculated in 2009 with ASTEC V2.0).

8 PLANT APPLICATIONS

8.1 GENERAL CAPABILITIES

The ASTEC V2.0 version can simulate all types of scenarios for PWR and VVER reactors in both usual power states and shutdown states. However, for the latter, some consolidation will be probably needed in the next months, due to the insufficient feed-back, at the present time, of the ASTEC use under such particular conditions; indeed, the CESAR operability on shutdown states situations has been demonstrated yet at IRSN through preliminary PWR 1300 MWe applications, but some improvements are expected as a feed-back from the validation against CATHARE results which is planned to be done by the end of 2009.

As concerns Gen.III reactors, preliminary applications were also performed on the EPR core catcher.

For CANDU reactors, most models are already applicable, mainly for fission products and containment phenomena but work is necessary for model adaptation to the primary heat transport system and especially for core degradation due to the horizontal core geometry.

For BWR reactors, the situation is similar: the efforts must focus in priority on model adaptation to the core degradation and then on RCS thermalhydraulics.

Most safety systems and SAM (Severe Accident Management) measures for the existing PWR and BWR can be represented: volunteer primary circuit depressurisation, steam generator management, spray system and venting in the containment.

8.2 TESTING CONDITIONS BEFORE V2.0 RELEASE

Before its freezing and delivery, the ASTEC V2.0 version has been applied by the ASTEC team to several sequences (most of them correspond to the delivery test-cases that are on the CD-ROM for version release [ref-44]) on different types of reactors:

- 4 complete sequences on French PWR 1300 MWe, coupling all modules: Loss of Steam Generator Feed-Water, Station Black-Out, Medium (6 inches diameter) Break LOCA (Loss Of Coolant Accident) and Small Break LOCA (0.6 inch diameter) in cold leg,
- 4 complete sequences on French PWR 900 MWe, also coupling all modules except ISODOP: Loss of Steam Generator Feed-Water, Station Black-Out, Medium (6 inches diameter) Break LOCA (Loss Of Coolant Accident) and Small Break LOCA (0.6 inch diameter) in cold leg; moreover, for two of them, a variant has been also tested in addition to the base case, changing the conditions of the hydro-accumulator discharge,
- 2 sequences on VVER-1000 (high-pressure and low-pressure scenario) coupling the CESAR, ICARE, ELSA, SOPHAEROS and CPA modules, i.e. without ex-vessel modules,
- 1 sequence on VVER-440, also coupling the CESAR, ICARE, ELSA, SOPHAEROS and CPA modules, i.e. without ex-vessel modules,
- 1 complete sequence on German Konvoi 1300 MWe (MBLOCA), only coupling the CESAR, ICARE and CPA modules, i.e. without ex-vessel and FP modules,
- 1 sequence on Westinghouse 1000, only coupling the CESAR and ICARE modules, i.e. limited to RCS thermalhydraulics and core degradation,
- The TMI-2 accidental scenario, only coupling the CESAR and ICARE modules, i.e. limited to RCS thermalhydraulics and in-vessel degradation,
- 1 additional complete sequence on an fictitious NPP-type, coupling all modules during a whole transient sequence, specifically devoted to test the ex-vessel corium behaviour in a core catcher configuration (fictitious input deck just created for V2.0 testing and roughly built from the combination of the in-vessel part from a fictitious PWR1300-like reactor and the ex-vessel part from a fictitious EPR-like reactor).

However, except for the TMI-2 case, it has to be underlined that, though globally representative of the NPP design they fit on, **these input decks have to be considered as simplified ones and in no way as best-estimate ones** (no efforts to optimise the RCS discretisation in CESAR, no activation of the 2D magma model in ICARE, …). **It means that these delivered data-sets have never to be used to perform safety analyses**.

In order to illustrate how a reference input deck should be structured, an additional CESAR/ICARE/CPA input data has been especially developed at IRSN on the general basis of a French PWR design (to be identified in the following as “pwr-like” input data). Using this delivered “pwr-like” input deck, two series of 4 sequences (the first one using in ICARE the 1D CAND model and the second one using the 2D MAGMA model) have been successfully calculated by the IRSN ASTEC team with ASTEC V2.0, up to the vessel failure occurrence. However, to prevent any misuse of this file, it has to be pointed out that, the true PWR input decks being private (IRSN property), this delivered CESAR/ICARE/CPA input data has to be interpreted as a kind of high-quality “pwr-like” input deck and in no way as a best-estimate “real” PWR input deck. In summary, **as far as the in-vessel processes are concerned, this additional “pwr-like” input deck shall be used by users as a good example for how a best-estimate NPP input deck should look like, while being never used as “black box” to perform reference PWR safety analyses**.

As concerns especially the front-end phase of a severe accident, ASTEC fully benefits also from the important series of benchmarks which have been achieved between CESAR and CATHARE V2.5 on the basis of the best-estimate “real” PWR-1300 input data [ref-58] [ref-59]. Indeed, very good results have been obtained with ASTEC for 14 different sequences, especially selected to be representative of the 6 main families of severe accident scenarios (LOCA, Station Black-Out, Loss of Steam Generator Feed-Water, Main Steam Line Break, Steam Generator Tube Rupture and, finally, Steam Generator Tube Rupture combined with a Main Steam Line Break).

As concerns the numerical stability and reliability of the ASTEC V2.0 version, the analysis of portability of the code has continued on several computer platforms (PC/Linux, PC/Windows) and with several different compilers.

In addition, as concerns the ASTEC suitability for PSA-2, the ASTEC V2.0 version fully benefits from the intensive use at IRSN and GRS of the latest ASTEC V1.3-rev2 version in the respective frame of the IRSN

PSA-2 on French PWR 1300 MWe and GRS PSA-2 consolidation work on German KONVOI 1300 MWe PWR.

8.3 FUTURE APPLICATIONS

As for the code assessment against small-scale experiments, it has to be underlined that, within the next 12 months, most of the plant applications which were performed in 2008 in the SARNET frame (through benchmarks exercises between ASTEC V1.3-rev2 and other integral codes such as MELCOR and MAAP4 [ref-60]) will be repeated soon using the V2.0 version in the particular frame of the SARNET phase 2 project. Moreover, other benchmarks are also planned to be done in the next months by non-SARNET partners such as, for instance, ASTEC-to-ICARE/CATHARE comparisons at Kurchatov Institute or comparisons at BARC of selected ASTEC stand-alone modules with dedicated Indian codes.

Finally, PSA-2 on the EPR reactor should start in 2009 at IRSN, using the ASTEC V2.0 version.

9 FUTURE AXES OF DEVELOPMENT

A first revision of ASTEC V2.0 (to be identified V2.0-rev1) is planned for the 1st part of 2010. This future V2.0-rev1 version should mainly account for the feedback of ASTEC V2.0 applications to be performed in 2009 in the frame of the SARNET phase-2 network, for the feedback of the code maintenance activities as well as for the last steps of the IRSN PWR-1300 and GRS KONVOI-1300 PSA level-2 studies. In addition, the reliability of the CESAR applications (and more generally the CESAR/ICARE/CPA operability) on shutdown states situations should be improved thanks in particular to some CESAR-to-CATHARE comparisons which are planned at short term at IRSN. In addition, efforts will be paid to further consolidate the ASTEC capability to simulate the in-vessel melt retention concept for some Gen.III new designs.

Moreover, besides these expected feed-backs, few modelling improvements should also be implemented in this future V2.0-rev1 version. These main modelling efforts in the next 6 months will concern the extension of the ICARE-MEDICIS coupling to the thermal behaviour of the lower head wall (after the lower head failure, the evaluation of the ICARE vessel wall temperature will account for the ex-vessel heat transfers, i.e. for the radiative heat fluxes issued from the corium located in the cavity).

As concerns user tools and user-friendliness, some efforts will continue to make easier both the pre-processing and post-processing of the code applications. For the latter, a new approach to couple the ATLAS tool to ASTEC was recently developed by GRS and IRSN; this new coupling methodology is now under testing at GRS, so that it could then replace the current one in the V2.0-rev1 version if it is proved to fully answer the main ATLAS requirements. In addition, the applicability of the ATLAS tool should be progressively extended to colour graphics for some other European reactor types, such as French PWRs, VVER-440 or EPR. Moreover, the ASTEC/KANT coupling (automatic coupling with dynamic PSA-2 methods) will be further tested and the use of the ASTEC/SUNSET coupling to evaluate the influence of uncertainties on data or models on the results should be intensified.

Finally, as for the MARCUS tool, a new ASTEC web site should be created (to become available by the end of 2009 at the "www-astec.irsn.fr" web address), aimed at making easier for users the download of either ASTEC load modules (patch versions, code revisions, …) or updated code documentation.

In parallel, the preparation of the second major ASTEC V2 version (to be identified V2.1) will start in 2009 and progressively intensify at IRSN and GRS up to its freezing and delivery which is expected end-2010.

The main modelling improvements to be implemented in the V2.1 version will concern a complete kinetics of chemical reactions in gaseous phase, an extension of the MDB library to most of the ASTEC modules (CESAR, ICARE, CPA, RUPUICUV), an update of the reflooding model for quasi-intact cores (to be transferred from the IRSN ICARE/CATHARE V2 code) and a first series of ASTEC adaptations to BWRs and CANDUs (mainly in the ICARE module), the latter taking in particular advantage of the new CESAR-ICARE coupling technique described hereafter.

Indeed, on a code structure point of view, one significant V2.1 evolution will concern the modification of the CESAR-ICARE coupling technique, thus allowing CESAR to cover the thermalhydraulics in the whole RCS (vessel and loops) during the whole transient (the switch to ICARE at the end of the front-end phase which was proved to have some drawbacks will be therefore suppressed). Besides, a 2D extension of CESAR will be also developed to support a radial discretisation of the core region as in ICARE, thus accounting for in-core 2D flow patterns.

Thanks to this new CESAR-ICARE coupling, the transport of any number of non-condensable gases in the core region during the in-vessel degradation phase will become possible (the in-core thermalhydraulics will be fully treated by CESAR during the core degradation phase, so that the current ICARE2 Zry/air oxidation model could be activated in ASTEC); that means the V2.1 version will allow to entirely simulate the situations of air ingress, either after vessel lower head rupture or during mid-loop states.

Moreover, in the frame of the SARNET phase-2 network, the integration into ASTEC of physical models will go on for the key-safety issues that remain open, such as in-vessel and ex-vessel corium coolability, and kinetics of iodine chemistry in the circuits. The feedback from the interpretation of the current experimental programs performed in the international frame will be taken into account in permanence: iodine chemistry in RCS and in containment (respectively CHIP and EPICUR at IRSN); heat flux spatial distribution in the corium pool during MCCI (VULCANO at CEA, OECD-CCI); effect of high fuel burn-up and of MOX fuel on core degradation and FP release (VERCORS then VERDON at CEA), ...

Finally, as concerns the ASTEC adaptation for other types of applications, both the modelling and assessment activities will go on, covering in particular HTGR (High Temperature Gas-cooled Reactors) investigations, accidents in ITER Fusion facility [ref-61] and use of some ASTEC modules for the IRSN emergency response tools (the latter work will lead to an acceleration of ASTEC computations and could imply a future extension to SA simulator tools)

As concerns long-term modelling activities, such as modelling issues on reflooding of severely damaged cores, they will progress in parallel in strong interconnection with the SARNET phase-2 work-package on the in-vessel corium coolability, using in particular the future data to be produced by the IRSN PEARL experimental programme.

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11 APPENDIX 1 : VALIDATION MATRIX

Table 1 : Matrix of ASTEC V2 basic validation for **CESAR and ICARE modules**

ASTEC V2 Basic validation matrix (rev.0)	BETHSY 9.1b *ISP27*	PACTEL *ISP33*	CORA 13 *ISP31*	CORA W2 *ISP36*	PHEBUS FPT4	LOFT-LP FP2	TMI-2	PHEBUS FPT1 *ISP46*
	CET	CET	CET	CET	CET	IT	IT	IT
CESAR								
Critical flow rates	D, M	M					D, M	
Inter-phase friction	D, M	M				D, M	D, M	D, M
Wall friction	D, M	M				D, M	D, M	D, M
CCFL								
Fluxes to walls	D, M	M				D, M	D, M	D, M
Condensation with incondensables						D, M	D, M	D, M
Horizontal SG (VVER)		M						
Core reflooding						M	M	
ICARE								
Core thermalhydraulics						D, M		
Core reflooding			D, M			M	M	
Clad ballooning						D, M	D, M	D, M
Ag-In-Cd control rods			D, M			D, M	D, M	D, M
B_4C control rods				M				
Oxidation						D, M	D, M	D, M
Eutectic melts						D, M	D, M	D, M
Fuel dissolution			D, M	M		D, M	D, M	D, M
Ceramic melts						D, M	D, M	D, M
Particulate debris			D, M		M	D, M	D, M	
Molten pool					M	D, M	D, M	D, M
Crust failure							D, M	
Structure ablation							D, M	D, M
FP release and transport						D, M	D, M	D, M
Corium slumping into the lower head							D, M	
Lower head failure								

D : Test which belongs to the "Delivery test-cases matrix"

M : Other tests belonging to the "Minimum validation matrix"

Table 2 : Matrix of ASTEC V2 basic validation for **ELSA and SOPHAEROS modules**

ASTEC V2 **Basic validation matrix (rev.0)**	VI-4	VERCORS 4	VERCORS 5	PHEBUS FPT4	TUBA TD07	TRANSAT TR04	FALCON 18	STORM SD-SR11 *ISP40*	ARTIST AR-PR5 E04/E06	PHEBUS FPT1 *ISP46*
	SET	SET	SET	CET	SET	CET	CET	CET	CET	IT
ELSA										
Volatile FP	D, M	D, M	M							D, M
Low-volatile FP	D, M	D, M	M	M						D, M
No-volatile FP				M						D, M
Control rod materials										D, M
Structural materials				M						D, M
Debris bed				M						
Molten pool				M						D, M
SOPHAEROS										
Aerosols settling							D, M			D, M
Laminar diffusion										D, M
Turbulent diffusion						M		D, M		D, M
Eddy impaction						M				D, M
Bend impaction						M				
Thermophoresis							D, M	D, M		D, M
Diffusiophoresis					D, M			D, M		D, M
Vapor FP condensation on walls							D, M			D, M
Vapor FP condensation on aerosols							D, M			D, M
Revaporisation								D, M		D, M
Chemi-Sorbtion							D, M			D, M
Mechanical aerosols resuspension								D, M		
Vapour chemistry							D, M			D, M
Homogeneous nucleation										D, M
Heterogeneous nucleation										D, M
Pool scrubbing on SG flooded secondary side									M	

D : Test which belongs to the “Delivery test-cases matrix”

M : Other tests belonging to the “Minimum validation matrix”

Table 3 : Matrix of ASTEC V2 basic validation for **CPA module**

ASTEC V2 Basic validation matrix (rev.0)	HDR E12.3-2	VANAM M3 *ISP37*	BmC Gx4	KAEVER 187 *ISP44*	CSE A10	EREC T5	TOSQAN MISTRA *ISP47*	PHEBUS FPT1 *ISP46*
	CET	CET	SET	CET	CET	CET	CET	IT
CPA-THY								
H_2 Combustion	D, M							
Passive Autocatalytic Recombiner			M					
Temperature distribution	D, M	D, M	M		M		M	D, M
Light gas distribution		D, M	M		M	M	M	D, M
Steam distribution		D, M	M		M	M	M	D, M
Convection pattern		D, M	M		M	M	M	D, M
Steam condensation on wall		D, M	M	M	M	M	M	D, M
Sensible heat transfer	D, M	D, M	M	M	M	M	M	D, M
Spray system					M		M	
Sump evaporation					M			D, M
FP decay heating								D, M
Boiling								
Bubble condenser tower (VVER-440)						M		
CPA-AFP								
Aerosols agglomeration		D, M		M				D, M
Aerosols sedimentation		D, M		M				D, M
Aerosols diffusion deposition		D, M		M				D, M
Aerosols diffusiophoresis		D, M		M				D, M
Condensation on aerosols		D, M		M				D, M
Condensation on hygroscopic aerosols		D, M		M				D, M
Multi-component effects		D, M		M				
Turbulent diffusion								
Resuspension								
Aerosol removal by spray					M			

D : Test which belongs to the "Delivery test-cases matrix"

M : Other tests belonging to the "Minimum validation matrix"

Table 4 : Matrix of ASTEC V2 basic validation for **RUPUICUV and MEDICIS modules**

ASTEC V2 **Basic validation matrix (rev.0)**	ANL U2	ANL IET 1RR	DISCO FH-02	ACE L2	BETA 2.3	OECD CCI2
	CET	SET	CET	CET	CET	SET
RUPUICUV						
Prototypical corium	M					
H_2 burning	M					
Corium entrainment	M	D, M	M			
Cavity water mitigation.						
Annular gap			M			
MEDICIS						
Zirconium content						
R H C upper surface					M	D, M
1 layer (mixed metal-oxide)				D, M		
Stratified corium (2 layers oxide/metal)					M	D, M
2D ablation					M	D, M
Siliceous concrete					M	
Limestone sand concrete				D, M		D, M

D : Test which belongs to the "Delivery test-cases matrix"

M : Other tests belonging to the "Minimum validation matrix"

Table 5 : Matrix of ASTEC V2 basic validation for **IODE module**

ASTEC V2 **Basic validation matrix (rev.0)**	PHEBUS RTF1 *ISP41*	PHEBUS RTF6	**ThAI** Iod12	CAIMAN 9 7/02 *ISP41*	CSE A10	PHEBUS FPT1 *ISP46*
	CET	CET	**CET**	CET	CET	IT
IODE						
Thermal reactions in water (sump)	D, M	M		D, M		D, M
Radiolytic reactions in sump	D, M	M		D, M		D, M
Reactions Ag/I in sump		M				D, M
Radiolytic reaction in gas (atmosphere)	D, M	M				D, M
Organic iodides	D, M	M		D, M		D, M
Sump-gas volatile species mass transfer	D, M	M	M	D, M		D, M
Deposition on surfaces (paint, steel…)	D, M	M	M	D, M		D, M
Steam condensation on walls		M	M			D, M
Boiling sump		M				
Particulate iodine behaviour		M				
pH in sump						
Iodine removal by spray					M	
Multi-compartment aspects			M			

D : Test which belongs to the “Delivery test-cases matrix”

M : Other tests belonging to the “Minimum validation matrix”

12 APPENDIX 2 : FIGURES

Fig.1 : Schema of the ASTEC V2.0 modules and of the code structure and running mode

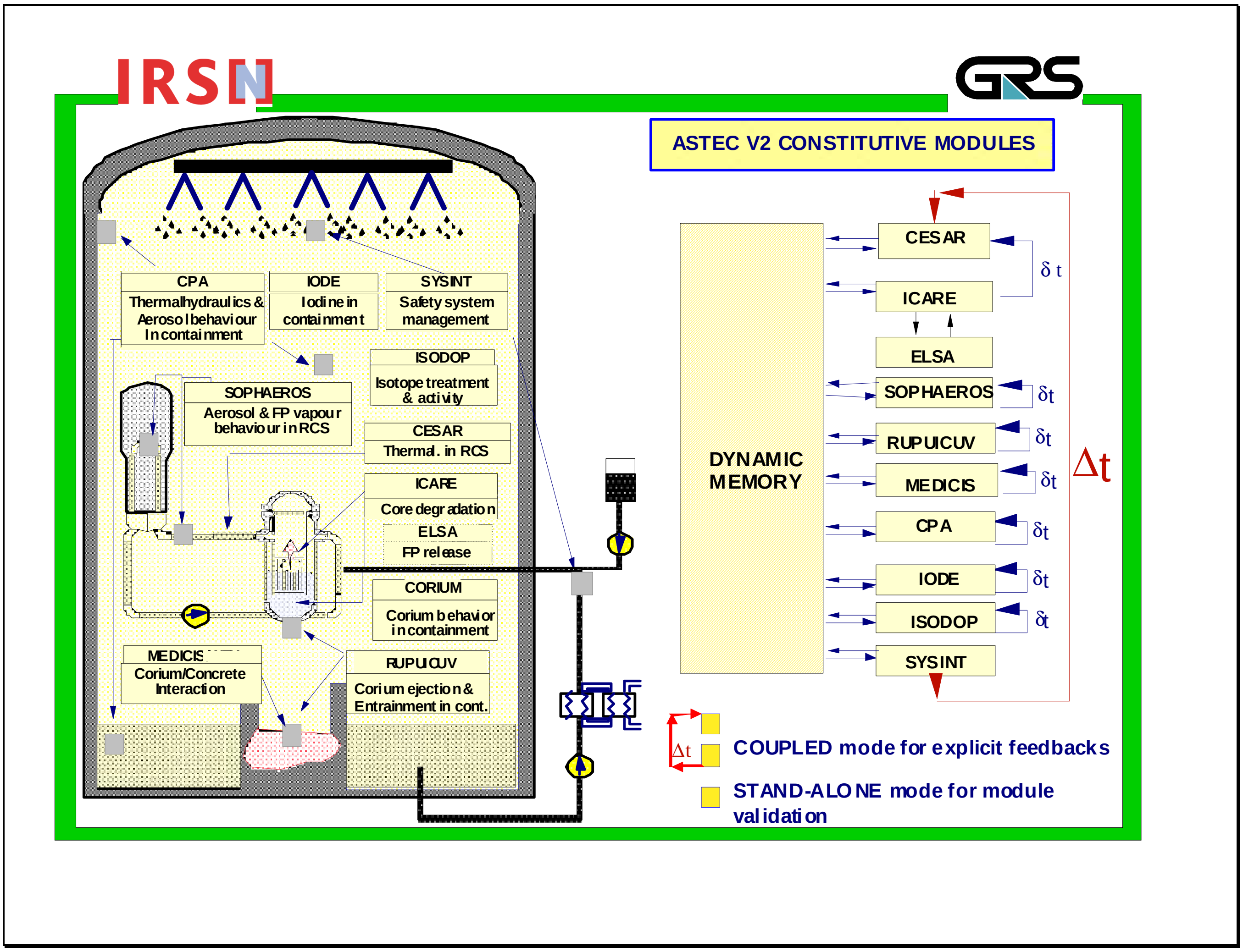

Fig.2 : CESAR-ICARE/MEDICIS coupling technique in ASTEC V2.0