Overview of ASTEC integral code status and perspectives

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ABSTRACT

The European severe accident integral code ASTEC, developed by IRSN, aims at simulating the progression and consequences of severe accidents (SA) in a water-cooled nuclear power plant (NPP). In particular, in France, the current ASTEC V2 series version are and will be in the next five years intensively used to perform deterministic and probabilistic safety analyses addressing the lifetime extension of the French operating fleet and the start-up of the EPR. This version is also used for emergency preparedness and response purposes. The benchmarking activities with MELCOR and MAAP on the Fukushima Daiichi accidents within the frame of the BSAF OCDE project evidenced significant discrepancies between SA codes likely to affect SAMG assessment. To deepen SA codes benchmarking, so-called crosswalk activities are conducted to identify needed SA models enhancement for consolidation of SAMG assessment. These discrepancies are related to the complex modelling of the fuel degradation and relocation that includes coupled thermodynamic, thermal mechanic and thermal hydraulic processes and that is currently revisited in a coordinated way by the leading SA code development teams (USNRC/SNL, EPRI, IAE and IRSN).

The elicitation of the SA modelling, its validation through dedicated and assessed experimental databases and its benchmarking on large sets of reactor configurations are the sound bases of SA codes. They will stay a subject of research and development at IRSN and they will be strengthened for ASTEC V2.1 by the users’ community through the NUGENIA ASCOM project coordinated by IRSN that started in autumn 2018.

These bases are the pillars for the innovative trajectory of development of the next ASTEC series of versions that just started in 2019, named ASTEC+, with two main objectives:
- to develop capacities to address any nuclear facility (NPP, spent fuel pool, fuel cycle facilities, material testing reactor, small modular reactor, Gen. IV concepts, nuclear fusion reactors…) and related risks,
- to streamline and to pool the efforts in the safety evaluation chain: deterministic evaluations plus uncertainties, level 2 Probabilistic Safety Analyses, emergency preparedness and response, SA desktop simulator.

Meeting these objectives at short term implies to reconsider globally the SA code development approach that was designed more than two decades ago to drastically improve the extendibility, the reusability, the verifiability and the ease of use of the code. IRSN has thus designed a new approach based on solutions that demonstrated their efficiency in various engineering contexts
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(object development, agile methods, advanced algorithms, high fidelity informed low fidelity models, surrogate models).

KEYWORDS
ASTEC, severe accident, computer code, validation

1. INTRODUCTION

Since 2016 The ASTEC code (Accident Source Term Evaluation Code) is developed by the French Technical Safety Organization “Institut de Radioprotection et de Sûreté Nucléaire”. It aims to model the entire accident sequence developing in a nuclear power plant, from the initiating event until the release of nuclear material in the environment, including the accident management response.

It has been developed initially to represent the pressurized light water reactors and has been enriched gradually to cope with other designs such as boiling water reactors, to some extents pressurized heavy water reactors and experimental facilities, including ITER fusion facility.

The last released version V2.1 has become the reference version for the severe accident safety studies performed at IRSN. It has been thus intensively used to assess the proposals of EDF to extend the lifetime of the French nuclear power plant fleet beyond forty years. Moreover, ASTEC is currently intensively used to contribute to the level 2 Probabilistic Safety Analysis relative to 900 MWe, 1300 MWe reactors and the upcoming EPR generation III+ reactor. It is also used for the assessment of source term evaluated by EDF.

In addition, ASTEC is the reference code among the European severe accident research community. Benefiting from the outcomes of European CESAM FP7 project [1] and in particular of the availability of generic datasets for each design of nuclear power plant represented in Europe, its assessment continues today through the recent project ASCOM led by IRSN in the NUGENIA frame and aiming to promote the use of ASTEC within the users community. Moreover, some important improvements have been done in the frame of the European H2020 IVMR project [4] and allow today the users to benefit from the state of the art models to assess long term in-vessel melt retention.

Concerning its validation, ASTEC is being continuously assessed using the latest results of research and development, integrating new results in order to remain the repository of the knowledge related to severe accident phenomena. Recent works have for instance been performed to validate the models for thermal hydraulic flows flowing through porous media in-vessel, for the vessel external cooling circuit in IVMR as well as for the top quenching during MCCI. Extreme conditions arising in severe accident limit dramatically the availability of relevant experiments and prevent classical validation approaches. As a consequence, in-depth benchmarking activities are crucial to increase the confidence in the code capabilities. In particular the OECD/BSAF projects (phase 1 and phase 2) have allowed comparing ASTEC results with other SA codes as well as measures and observations realized by Fukushima Daiichi operator TEPCO. These comparisons have been pursued in a more in-depth inter-codes exercise leading to the crosswalk between ASTEC and MELCOR.
Meanwhile the V2 current series of ASTEC versions will remain the reference version used in the next five years. The IRSN has just launched in parallel the ASTEC+ trajectory, a new pathway for the development of ASTEC aiming to extend its capabilities to uncovered scenarios and facilities, addressing the source term evaluation whatever the facility. In this context, the software development in various domains will employ improved code development technics, already successfully widespread implemented software, and new algorithms in order to increase the extensibility, the sustainability, the reliability, the modularity and the efficiency of the code.

2. EXAMPLES OF ASTEC USE FOR SAFETY STUDIES AT IRSN

In this chapter, some of the use cases of ASTEC V2.1 at IRSN are described. The examples are related to the mission of IRSN in France which consists in technical expertise of requests formulated by utilities (often EDF) to French authorities, represented by ASN.

2.1. Extension Of Plant Fleet Lifetime

In order to extend the 900 MWe plants lifetime beyond 40 years, EDF, the French utility, has made the decision for upgrading severe accident mitigation with significant modifications proposed for two objectives:

- avoiding concrete basemat melt-through by melted core after vessel failure;
- avoiding containment over-pressurization and venting by addition of a new system to remove residual heat out of containment.

EDF has performed MAAP4 and TOLBIAC-ICB (c.f. [2]) simulations to demonstrate the efficiency of these modifications and IRSN uses ASTEC V2.1 simulations to support its assessment of EDF proposals.

Concerning MCCI simulations, IRSN has calculated MCCI under water, taking into account the plant modifications providing additional corium spreading area and early passive top-flooding EDF is planning to implement, for different concrete basemat compositions (see Figure 1 b) c)). As result, some differences on the calculated ablated thicknesses of the concrete basemat were obtained, depending on concrete composition.

Concerning the new system to remove residual heat out of containment, this system is relying on a fixed heat exchanger, and a mobile cold source to be lined by the EDF rescue team during crisis management. The main issue is that the installation needs to have a sufficient “grace period” for the reaction time of the EDF rescue team to install the mobile cold source in due time to avoid containment over-pressurization and with large enough safety margins.

IRSN has modeled this new system through ASTEC V2.1 (pump, injections lines, heat exchange represented in Figure 1 d) and has conducted a series of calculations in order to evaluate the grace period available and the performance of the heat exchanger, once the cold source is connected. Several scenarios were simulated with ASTEC V2.1 such as the total loss of electrical power supply and cold sources (like for Fukushima-Daiichi accident) or the loss of coolant accident evolving into a severe accident. These simulations were performed to assess the progress of these accidents taking into account the new system with a particular interest concerning the evolutions...
of the containment pressurization as well as the temperature of the water circulating in the new system.

![Figure 1](image)

**Figure 1** Schematic representations of different phases of stabilization of corium ex-vessel modelled with ASTEC: a) slump from vessel to dry cavity b) spreading in dry cavity and dedicated adjacent room c) top flooding of corium by water d) ultimate residual heat removal circuit

### 2.2. Source Term Assessment

The ASTEC code has been used for several years to assess the source term released in the environment through controlled and uncontrolled leaks in case of a nuclear accident. These evaluations are used at IRSN for the safety review analyses, and for internal uses such as crisis management or level 2 probabilistic safety assessment activities. Recently, within the scope of the fourth decennial reactor safety reviews for the French 900 MWe nuclear power plants, the current ASTEC version has been used intensively to perform source term evaluations. In addition to study the impact of the latest R&D results on the source term, the goal was twofold. The first goal was to check the order of magnitude of the source term assessed by the operator. The second goal was to make sure the post-Fukushima Daiichi complementary safety assessments and related plant modifications lead to reduce the source term in the event of a nuclear accident. Many ASTEC calculations have been made to fulfill these objectives. In particular, a large number of sensitivity analyses have been carried out to evaluate the uncertainties on the results, especially concerning the iodine chemistry. As an example, the figure below highlights the influence of the boiling sump hypothesis on the molecular iodine mass released from the sump to the gas.
2.3. State Of The Art Source Term Modeling

The ASTEC code capitalizes the entire R&D performed at IRSN for several years that addressed the different phenomena involved in the FP release to the environment. First-of-all as concerns the FP release from core, the strategy is to improve the understanding of these complex phenomena using mechanistic codes such as MFPR, ASTEC benefiting from these results with the simplified module ELSA.

Second-of-all, the R&D in FP transport was driven by a better understanding of the gaseous fraction measured at the break during the Phebus FP experiments. This gaseous fraction was not explained initially and the last decade was dedicated to better understand iodine interaction with other FP such as Cs or Mo in the RCS. The ASTEC code capitalizes this R&D performed in the framework of several program such as ISTP and STEM (see [3]) and with university collaboration (C3R). Today, current investigations concern the ruthenium chemistry and the interactions between iodine and control rods elements (Ag, Cd, B) which has still to be consolidated.

Third-of-all, concerning FP chemistry in the containment, the R&D is still ongoing (see next paragraph). Nevertheless, a better understanding of the iodine chemistry is obtained capitalizing all the experiments performed in STEM, BIP and THAI programs. Considering a quite good understanding of the aqueous phase phenomena has been reached, the R&D is focusing now on phenomena in the gaseous phase, especially on iodine oxide behaviour on the long term (decomposition, interaction with other aerosol) and organic iodine formation with other organic compounds.

In conclusion, ASTEC is able today to compute a source term taking into account the most relevant and recent R&D performed from the FP core release to the FP release from the containment.
3. ASTEC AND THE R&D ON SA

In this chapter are described the R&D topics which are currently under investigation at IRSN and which are addressed by the development of new features of ASTEC.

3.1. IVMR Outcomes

The IVMR project is a European project launched in the scope of the EU Research and Innovation program Horizon 2020. It aims at providing new knowledge (experimental, theoretical and technical) and a new methodology providing a best-estimate evaluation of IVR strategy for large power reactors. This project started in 2015 and will be completed at the end of 2019. It initially gathered 23 European organizations (Utilities, Technical Support Organizations, Nuclear Power Plant vendors, Research Institutes...) and several new partners from Korea, China, Russia, Japan and Ukraine were integrated recently in the project. IVR strategy attracts a lot of interests either for new reactor designs currently under construction in the world (AP1000, APR-1400, HPR-1000) or as back-fitting measure to existing Gen. II reactors (especially for VVER1000 reactors in Europe).

The ASTEC code is used by several participants in this project, both for reactor simulations and modelling tasks. Regarding the first task, ASTEC was widely used in the first set of reactor calculations performed at the beginning of the project for various reactor designs (PWR, VVER440 and VVER1000) by 7 different partners. The results obtained showed the capabilities of ASTEC to simulate IVR strategy, provided that the vessel wall meshing is sufficiently refined and mechanical models designed for situations without external cooling are disabled. More generally, this first set of reactor calculations allowed identifying the high impact of design parameters such as the ratio of the mass of fuel to the mass of steel that is likely to be molten in the lower plenum and the ratio of the mass of fuel to the cumulated mass of water in the vessel before a long term dry-out is reached [4]. The calculations have also shown that some transient phases may lead to high heat fluxes before the steady state configuration is reached. In particular, some of these situations arising after stratification inversion, i.e. when the previously heavy metal becomes lighter, appear to be the most critical. Those high heat fluxes may be much larger than the “steady-state” heat flux. However, they may not cause the vessel failure if they occur only for short time intervals. Therefore, it appears that the modelling of transient phenomena in the lower head is needed to conclude on feasibility of IVR strategy, at least for high power reactor when safety margins are reduced. This conclusion was confirmed and completed by the outcomes of the Phenomena Identification Ranking Table (PIRT) on IVR elaborated in the scope of the project [5].

In accordance with these conclusions, significant modelling improvements have been implemented in ASTEC V2.1.1 code in order to allow a better evaluation of transient situations. First of all, a new model for simulating the kinetics of corium pool stratification in the lower head was added. This model is described and illustrated in [5]. It is based on the results of MASCA experiments [7] for the thermochemistry in the corium pool and on CORDEB experiments [8] which recently studied the kinetics of stratification in the 3-layers configurations.
Figure 3 – a) Illustration of stratification inversion process and b) example of maximum heat flux profile along the lower head obtained at stratification inversion with ASTEC code compared to the flux evaluated at steady-state (from [5])

Further developments concern the boundary conditions at the top of the molten pool, with:
- The adaptation to lower head specificities of the existing corium pool oxidation model used in the core part of the vessel;
- The improvement of the model dealing with heat transfers with the water at the top of the corium pool (implementation of the boiling curve);
- The improvement of the radiative heat transfers evaluation in order to consider all the walls in the vessel cavity above the top surface of the pool and not only the core support plate as it was in the previous model.

Moreover, a finer modelling of the metal structures in the lower head (geometry, meshing) as well as for the meshing of the vessel wall has been proposed to users.

Concerning the external cooling circuit implementing IVR strategy, a new feature was developed in ASTEC allowing the simulation of the natural convective flow which establishes in the ERVC loop. A specific coupling between the vessel wall meshes modelled by ICARE module and the external water modelled by CESAR module has been implemented and validated [9].

Figure 4 – Example of ERVC simulation using ASTEC code

Finally an additional improvement allows ASTEC to deal with the situation where the lower plenum is over-filled with molten materials. Indeed, due to the discontinuity of models between
the core part and the lower plenum in ASTEC approach (2D modelling for core degradation and then 0D modelling for corium stratification), with previous versions of ASTEC when the lower head was full (long term situation for IVR, design with small lower plenum…) the models in the lower plenum (turbulent convective heat transfer, thermochemistry and phases separation…) did not consider the corium mass located in the core part (above the specified upper limit of the lower plenum region). This limitation has been overcome by an automatic and progressive extension of the lower head size as soon as it is full of materials.

Additionally, it is worth noting those new features are currently used by the IVMR partners in the last step of reactor calculations done during this last year of the project.

3.2. Debris Modelling

The reflooding of a degraded core is a key issue for safety: depending on the core state conditions at the reflooding time and on the water mass flow rate injected, it may be an efficient way to stop the progression of the accident or it may lead to further degradation with the creation of a debris bed and an increased hydrogen production. In this context, a modelling of in-core debris was implemented in ASTEC. It includes debris bed formation, oxidation and melting, debris relocation and a specific thermal-hydraulic treatment.

In the V2.1 version of the ASTEC code, the particles that result from the fragmentation and the collapse of solid structures during the degradation phase (especially in case of reflooding) are modeled by new DEBRIS components. These components aim at representing fragments of fuel pellets, claddings, grids and control rods with various sizes and shapes. Each type of debris is characterized by a mean diameter determined such that the surface area-to-volume ratio of the particle distribution is kept unchanged [10]. This is of fundamental importance for oxidation and coolability since it controls the rate at which a particle interacts with the fluid. The DEBRIS coming from fuel rod claddings can be oxidized and all DEBRIS components can melt and be converted into MAGMA once their melting temperature is reached, contributing to the formation of a molten pool.

One of the commonly accepted mechanisms for the creation of a debris bed is the collapse of damaged fuel rods during reflooding. It is assumed in ASTEC that the fuel pellets are fragmented from the first rise of power (base irradiation in normal operating conditions) [11] and generate debris if their surrounding claddings are either melted or highly embrittled and subjected to a thermal-shock (cooling rate greater than 5 K/s). The criterion for the cladding embrittlement during the oxidation process is based on the thickness of the beta-phase of Zircaloy (β-Zr), as it is usually done for LOCA conditions. Considering various data [12, 13], we have assumed that fuel rod cladding with a β-Zr layer thinner than 100 μm will fail in case of thermal shock to form a debris bed.

The DEBRIS components have also the ability to relocate in the core to progressively fill meshes. The relocation is based on a simple dynamic model assuming that debris in the reactor core behaves like grains flowing through an orifice based on the Beverloo law [14]. In addition, a blockage of debris components is assumed for porosities lower than 0.4 (due to arching effect).

Finally, the thermal-hydraulics module CESAR of ASTEC V2.1 has been extended from a five-equation model to a six-equation model in order to compute the thermal-hydraulics in the debris bed using two momentum equations [15]. This new set of equations is enabled only in porous
meshes, according to a criterion based on the dominant friction area (rods or debris). The friction terms are computed using classical expressions depending on the passability and permeability of the porous medium: the relative passability and permeability come from the Reed formulation while the absolute passability and the permeability are determined using the Carman–Kozeny and Ergun relations. The interfacial friction term is computed using the Schulenberg correlation [16]. A reflooding model [17], able to deal with any geometry including debris beds, is based on the detection of a quench front according to the fuel rod and/or debris temperature and the presence of water.

This in-core debris bed modelling has been used to compute the TMI-2 accident in order to assess its ability to simulate the progression of core damage, including the reflooding phase. The TMI-2 accident, which occurred in March 1979, is the first severe accident in a light water reactor. It resulted in extensive oxidation and melting of the reactor core, formation of a large debris bed and significant release of fission products from fuel. In spite of severe core damage, water in the reactor vessel and continued high-pressure water injection prevented failure of the reactor vessel's lower head. Using both MAGMA–historical models of degradation of ASTEC considering the melting of materials- and new DEBRIS components in ASTEC computation implies a competition between their respective formation criteria that governs the final amounts of molten corium and debris.

Two modelling options for MAGMA formation have been therefore considered for the TMI-2 computation. The 1st option (reference case) uses the modelling choices recommended today for any reactor computations with ASTEC V2.1. They come from interpretation of the Phebus FP experiments [18] and aims at representing early fuel liquefaction processes. They consist in defining a lowered melting temperature for fuel rod materials (UO$_2$) and oxidized cladding (ZrO$_2$) (T$_{sol}$/T$_{liq}$=2550 K/2600 K) together with a loss of integrity for claddings with a zirconia thickness lower than 250 μm and temperature beyond 2300 K.

The 2nd option (alternative case) simply consists in keeping theoretical melting temperatures for UO$_2$ and ZrO$_2$, without any loss of integrity criterion. Criteria taken for DEBRIS formation are those described above.

The analysis of the reference case showed that thermal-hydraulics parameters such as primary pressure, pressurizer level and core collapsed level are well predicted during the degradation phase up to the re-start of the primary pump at 10440 s (instant of reflooding). The production of hydrogen is well reproduced until 10000 s, time at which an important fuel melting due to the
lowering of solidus/liquidus temperature of UO$_2$/ZrO$_2$ occurs. The oxidation kinetics being slower for molten and relocated materials than for standing rods, a strong decrease of the hydrogen production is observed with only 210 kg of hydrogen produced in the simulation against 450 kg in the accident (see Figure 5 a)). At the end of the simulation around 35 tons of molten materials and 10 tons of debris are located in the core without any debris/magma in the lower head (see Figure 5 b)). In comparison the analysis of the TMI-2 reactor core [19] gave 25 tons of molten materials, 30 tons of upper core debris and 16 tons of lower plenum debris.

The TMI-2 simulation performed in the reference case leads consequently to significantly smaller amount of relocated materials (45 tons) and lower hydrogen production (210 kg) comparing to the measured ones (71 tons and 450 kg respectively).

The second simulation (alternative case) highlighted that considering theoretical melting temperatures for UO$_2$ and ZrO$_2$ materials had a significant impact on the core degradation: the fuel rods and claddings keep their ‘intact’ geometry longer, staying available for oxidation, and reach therefore higher temperatures than in the reference calculation. In fact, the delayed loss of the rod-like geometry enhances strongly the oxidation kinetics, with more than 500 kg of H$_2$ produced (see Figure 6 a)). Here 72% of H$_2$ produced comes from claddings oxidation (28% from magmas) against 61% in the reference case. Finally, the Figure 6 b) shows that around 40 tons of magma and 60 tons of debris are formed in the core. Only 20 kg of corium is observed in the lower plenum.

This study put in evidence the possibilities offered by ASTEC V2.1 to describe more precisely the core degradation phase thanks to combining both DEBRIS and MAGMA components. It has also clearly shown the importance of the fuel assemblies’ loss of integrity criteria to convert solid components into MAGMA or DEBRIS components. More details concerning this study are available in [20].

3.3. Iodine chemistry in containment

ASTEC FP models have been modified significantly since 2013, especially for iodine chemistry in the gaseous phase. A new iodine-paint model was implemented in ASTEC V2.1 in 2015,[21, 22]. A preliminary model of gaseous organic iodides (RI) formation from the radiolytic reaction between volatile organic compounds (like C$_n$H$_m$) with molecular iodine has also been set up with few experimental data. It helps in predicting RI volatility in several tests [21]. It however needs to be completed with a complementary experimental approach.
More recently (2017), iodine oxides aerosols (IOx) decomposition has been studied in the framework of OECD-STEM and OECD-STEM2 projects. From these new data, a new IOx decomposition model has been set up in ASTEC V2.1.1.

For the sump, in alkaline conditions, the interpretation of PASSAM project tests highlighted that hypoiodous acid (HOI) volatility could be significant [23, 24]. HOI mass transfer from the sump to the gaseous phase was thus set up as a default reaction in ASTEC V2.1.1. As HOI gaseous chemistry is not known, HOI is automatically converted into gaseous I\(_2\) as soon as it reaches the gaseous phase.

In conclusion, all these improvements brought ASTEC code to the state-of-the-art regarding the iodine behavior in the containment, in the liquid part as well as in the atmosphere.

4. ASTEC COMMUNITY

4.1. ASCOM Project

The CESAM FP7 project in 2013-2017 [1] has been successfully conducted in EURATOM frame in the aftermath of the Fukushima Dai-ichi accidents, with two main goals:

- to achieve an improved understanding of all relevant phenomena during these accidents and their importance for SA Management (SAM) measures;
- to simultaneously improve the ASTEC V2.1 code to simulate plant behaviour throughout accident sequences including SAM measures.

However, though a significant modelling progress could be achieved, notably as regards Gen.II NPPs, IRSN came to the conclusion that all these efforts must be pursued for Gen.II, III & III+ NPPs. That’s a purpose of the ASCOM (ASTEC Commmunity) in-kind project (i.e. without any external funding, thus relying on partners’ own resources), led by IRSN, that started in October 2018 for a 4-year long duration under NUGENIA/SARNET Technical Area 2 (severe accidents).

Moreover, the ASCOM project aims at fostering the collaboration between all ASTEC users, on the basis of in-kind contributions to be distributed over several work-packages (WPs). The main objective is to help amplify and accelerate the on-going process of making the ASTEC code a fully reliable tool for SA analyses and accident management in a wide range of nuclear safety applications by strengthening the activities of this ASTEC community in a consistent way.

ASCOM is gathering 25 organizations worldwide: IRSN, CIEMAT, NUBIKI, KIT, Università di Pisa, ENEA, IVS, EDF R&D, Energorisk, FER, HZDR, IJS, INRNE, JRC, LEI, NRC-KI, NSC, NUS, RATEN ICN, RUB, SEC NRS, TRACTEBEL, UJV, University of Utah, VTT.

Within the ASCOM work programme, four “technical” work-packages (WPs) have been set-up:

- Improvements of ASTEC physical modelling and ASTEC overall capabilities (e.g. new models as necessary for Gen.III+ designs, spent fuel pools (SFPs)…), along with an IRSN support to ASTEC users;
- Continuous validation of ASTEC V2 models vs. Separate-Effect-Tests or Integral experiments;
- ASTEC applications at reactor scale through two main lines:
  - Consolidation/update of ASTEC V2 existing generic reference input decks for PWRs, VVERs and BWRs, all of which are relating today to Gen.II NPPs;
Follow-up of comparisons at plant scale between ASTEC V2 and other reference codes on selected SA sequences for all Gen.II NPP types operated in Europe today.

- Development of few new generic NPP and SFP reference input decks to extend the ASTEC applicability to other kinds of nuclear installations (Gen. III & III+ SMR, etc.).

The main expected outcomes of the ASCOM project are therefore

- Reinforcement of validation database;
- Consolidation of the existing V2.1 dataset library for generic Gen.II NPPs;
- Extension of this open generic dataset library to some new designs;
- Subsequent extension of the ASTEC V2 application scope, along with likely some further improvement of the ASTEC code reliability for SA analyses and accident management as a feed-back from the planned intensive use of ASTEC V2 by various partners.

5. BENCHMARK WITH RESPECT TO OTHER SA CODES

5.1. BSAF Project

In the frame of the OECD BSAF (Benchmark of Severe Accident code for Fukushima-Daiichī accident) project, was pursued the objectives of improving the understanding of what happened in the three units of the Fukushima-Daiichī power plant, improving the severe accident codes and preparing the decommissioning of the facilities.

The first step of the project was focused on thermal-hydraulics behavior and core degradation. IRSN participated with the previous version of ASTEC V2.0. This first part yielded the conclusions that the severe accident codes, despite their very different modelling, was quite coherent concerning the first stages of the accident but large discrepancies was observed concerning the advanced degradation (e.g. for H₂ production). These discrepancies lead to an in-depth analysis of differences between degradation models implemented by MELCOR and MAAP in the so-called MELCOR/MAAP crosswalk which was pursued by the same kind of analysis through the MELCOR/ASTEC crosswalk exercise described in the next paragraph.

The second step of the project between 2015 and 2018 continued on core degradation but also on the source term assessment. On this occasion, the V2.1 version of ASTEC bringing the up-to-date models of fission-transport was used.

It was quite difficult to agree on a final scenario for each unit because different leakage hypotheses can lead to the same kind of thermal-hydraulic evolutions. Nevertheless, this project allows stating several conclusions.

Firstly, there are uncertainties on the calculated release of several radioisotopes, in particular isotopes of Sr and Ba. Sr is of particular interest because Sr isotopes contribute significantly to the radiological effects today. In ASTEC, most part of calculated Sr and Ba release come from the molten pool and very few experiments exist to validate models for FP release from corium pools. These models will need to be reassessed.

Secondly, the global release regarding iodine and caesium can be reasonably well reproduced with the ASTEC code. However, amplitude and timings of release phases calculated by ASTEC
(direct calculations) are significantly different from release phase deduced from environment measurements (inverse calculations). These differences can be explained by uncertainties related to the accident development in each unit (uncertainties on direct calculations) and by uncertainties on calculations of FP dispersion in the environment (uncertainties on inverse calculations linked in particular to uncertainties on meteorological data). The comparison between direct source term calculated by SA code and inverse source term built from environment measurement will be furthered in the coming OECD/NEA ARC-F project to better understand the accident development in all three units.

Thirdly, if the global release is well reproduced, the long term release is not modelled by ASTEC code for all the elements. Because of detailed iodine chemistry description, the long term release of iodine is reasonably well computed but, essentially because caesium is considered as particle, after the settling of the aerosols, the code could not calculate the long term release of Caesium.

A simple hypothesis was to consider aerosol re-vaporization from RPV. One can be aware that retention in RPV can reach 50% of the initial inventory depending on unit. Re-vaporization of this retention can explain the long term release observed during the accident.

In Figure 7, a comparison of the global release of $^{137}$Cs and $^{131}$I is done between ASTEC source term and several source terms obtained by inverse methods (called “environment source term” afterward). We can notice firstly that the global released amount is quite consistent for all source terms. At the beginning of the accident, there is no consensus on release kinetics for environment source terms. The differences are due to differences in measurements and meteorological field used. For instance for $^{137}$Cs release, the orange curve (Sau) corresponds to [25] obtained using the ECMWF meteorological field. Brown curve (Sau1) is obtained using same dose rate measurements but the MRI meteorological field. Green curve (Sau2) is obtained using the MRI meteorological field and additional air measurements.

![Figure 7: $^{137}$Cs and $^{131}$I global release - comparison between ASTEC source term and environment source term (Kat: [26], Ter: [27], Sau: [25], Sau1: Sau+MRI, Sau2: Sau1+air measurement)](image)

Taking into account in ASTEC a non-physically-justified high level of re-vaporization of aerosols from reactor pressure vessel wall deposition, Figure 8 shows new calculated release rate for $^{137}$Cs and $^{131}$I. There is no major change for iodine because the main part of its chronical
release is due to chemistry but ASTEC now continues to compute release of Cs after 6 days. The order of the release rate is quite consistent with the release rate estimated with inverse methods.

![Figure 8: $^{137}$Cs and $^{131}$I release rate - comparison between ASTEC source term and environment source term with FP re-entrainment from liquid phase (Kat: [26], Ter: [27])](image)

5.2. ASTEC/MELCOR Crosswalk Study

The ASTEC/MELCOR Crosswalk study [28] was an in-depth code-to-code comparison undertaken by the SNL and IRSN developers of the severe accident codes to better understand the difference prevailing in the degradation models which explain mainly the difference in advanced degradation phenomena.

As the preceding MAAP/MELCOR study carried out by USNRC/SNL and EPRI, this advanced benchmark aimed to compare the response of the severe accident analysis codes on a stylized Fukushima-Daiichi Unit 1-like scenario.

In this way, the main events and assumptions of the scenario were the same for each calculation. Indeed, given the different code frameworks in both MELCOR and ASTEC, an effort was made to reduce as much as possible the differences in the problem geometry and the initial conditions at the point of core uncovering.

This work highlighted the importance of degradation models on final results. Indeed, before the first oxidation peak, the residual power is mainly evacuated by convection and the general agreement between the codes is observed. But during the degradation process, several models have been identified as source of discrepancies between the codes. For example, MELCOR treats debris as a combination of both particulate debris and molten debris. ASTEC treats degraded fuel as a unified field called “magma.” This “magma” field more closely resembles molten debris as opposed to the particulate debris predicted by MELCOR. In the uncovered part of the core, the increase in temperature is strongly driven by oxidation of Zircaloy. Accounting for the meltdown or the collapse of fuel rods has a significant impact on the calculation of temperatures. Therefore, ASTEC and MELCOR temperature fields are very different during core degradation (see Figure 9).
As the core degradation process proceeds, the “magma” formed in the ASTEC simulation leads to significant blockage of flow channels. As these channels become blocked, a minimum fraction is imposed to allow for chemical interactions such as oxidation to proceed. In contrast, the particulate debris predicted by MELCOR is much more porous. Additionally, as fuel assemblies collapse in MELCOR (not modeled in ASTEC) large areas of the core region become open to flow that were previously blocked by debris.

This analysis underlines the fact that severe accident analysis codes assume different effective morphologies (modeling abstractions) to describe and represent degraded core materials. MELCOR calculates the formation of primarily particulate debris with some molten debris. ASTEC calculates the formation of a pool mainly composed of molten materials, with a minimum gas flow area through the pool.

Those morphological representations directly impact the porosity and surface area of the debris, and thus have a significant impact on the coolability and oxidation of these materials. Accordingly, the thermal-hydraulic response can differ greatly at times between the two codes. It is worth noting that despite the fact that these codes can differ dramatically in thermal-hydraulic behavior, the overall oxidation predicted by the two codes does not differ significantly. Additionally, the time of lower head failure is also similar, even though the location of lower head failure is different.

Figure 9 comparison of core degradation between ASTEC and MELCOR in the frame of Crosswalk exercise on a stylized Fukushima-like accidental scenario: representation of fuel temperature in the core during degradation; dark zones represent zones freed by fuel melting
6. ASTEC+ PERSPECTIVES

ASTEC+ is an innovative trajectory within the ASTEC project which aims to design the future versions of ASTEC. The main goals of these new versions are:

- To address with ASTEC, depending on the associated risks, any nuclear facility (NPP, spent fuel pool, fuel cycle, material testing reactor, small modular reactor, Gen.IV concepts, nuclear fusion...),
- To streamline and to pool the efforts in the safety evaluation chain: deterministic evaluations plus uncertainties, PSA2, emergency preparedness and response, SA desktop simulator.

In this chapter, we will describe some key ingredients which will be required for this major evolution of ASTEC.

6.1.1. Architecture of ASTEC+

The first requirement of ASTEC+ is to ensure the compatibility with the current version of ASTEC.

This is actually a strong requirement which implies the compatibility of ASTEC+ with ODESSA format but it is imposed by the large number of existing datasets.

In order to guarantee this compatibility, the ASTEC+ initiative will proceed by adding some new modules in ASTEC which will be able to replace progressively the existing modules however extending their capabilities (see Figure 10).

Moreover, generic components of ASTEC+ will be developed in a framework (Severe Accident Framework, see Figure 11), independent of ASTEC, which will authorize these components to be used out of ASTEC, depending on their final use: crisis application, PSA 2 framework, simulator, etc.
ASTEC+ should benefit of the advantages of object oriented programming. This requirement implies the use of an efficient object programming language –the C++ language for ASTEC+- but it will be accompanied with strong object programming good-practices, essentially those promoted by agile methods and ensuring the best level of confidence and robustness in the software.

In order to benefit simultaneously from the experience in intensive numerical simulation as well as object programming good practices, ASTEC+ will be developed on the basis of PELICANS framework (c.f. [29]).

This framework has been developed at IRSN for the purpose of numerical demanding scientific applications such as CFD computation. From one side, it implements some features in numerical algebra, parallelism, geometry, finite element and finite volume resolution method which could benefit to ASTEC+, but moreover, PELICANS offers a framework of development which:

- Restrict the use of C++ to safest features of the language;
- Provide tools to implement object paradigms e.g. contract programming, test-driven development, automatic documentation, Liskov substitution principle rule…

### 6.1.3. Multi-scale and flexible approaches

One goal of ASTEC+ is to promote the multi-scale approach when detailed models are available to inform simpler models. This approach seems particularly valuable when detailed model are already available and used to solve problems which are solved in a simpler way in ASTEC. In fact, the general lumped parameter approach implemented by ASTEC generally leads to neglect
some phenomena (e.g. the viscosity of fluid) or to roughly approximate some others (parietal friction laws). The domain of application with ASTEC+ can be large, e.g.:

- A Computational Fluid Dynamic code solving multiphasic flows as the IRSN *MC3D* code [29] can be used to refine the thermal-hydraulic phenomena in the Reactor Cooling Circuit, particularly when the lumped parameter approach is no more sufficient to describe the relevant physics (complex flows, multidimensional pattern, mixing, etc.) or when extreme conditions arise (e.g. during Corium-Water Interaction),
- In a same way, fire and dispersion CFD code as the IRSN code *PREMICS* [31] can be used to refine the behavior of gases in the containment, as instance as concerns the hydrogen dispersion and combustion which are hardly represented by lumped-parameter models of ASTEC/CPA module,
- When thermal-dynamic properties of a corium-based mixture is of interest, as instance for in-vessel or ex-vessel speciation, the *NUCLEA* database [32] developed at IRSN can replace the simpler model implemented in MDB library today;
- Thermal-mechanical code can be used to determine the rupture of the circuit.

The strategy will consist to consider preferably the codes developed at IRSN and to implement a two-step approach. In the first step, the external coupling between ASTEC and the detailed code will be tested and assessed with respect to available experiments. In a second step and if relevant, the coupling between the integral code ASTEC and the detailed modelling will be performed.

This last step of coupling represents an example of the flexible approach. Here the flexible approach means that different kind of discretization can be applied on the same set of phenomena. For instance in the multi-scale frame, a lumped parameter model can be adjoined, in one specific zone, to a full discretized model. But the flexible approach comprises also the availability of the code to solve explicitly or implicitly coupled problem. In both cases, the modelled objet is the same, but the discretization as well as the numerical methods are completely different. As example, the coupling between MCCI phenomena and containment atmosphere is explicitly coupled in ASTEC: it means that each module does its calculations separately and the coupling arises at the end of time step, when each module read the result of preceding ones. But we can imagine that in case of strong coupling, it would be necessary to solve simultaneously both set of phenomena: the versatility allowing switching easily from an explicit to an implicit scheme is an illustration of flexible approach.

### 6.1.4. Advanced algorithms

ASTEC+ trajectory will promote the use of advanced algorithms popularized these last years by numerous applications.

Among these algorithms, we have identified the following that can be used in our applications:

- Surrogate model: these models are generally informed by higher level of fidelity models to provide a simpler and quick response. Actually, the objectives along ASTEC+ if simultaneously to implement generic methods allowing to generate such model, but also to use these models in replacement of more complicated model for specific purposes (in a multi-scale approach). These models aim to “condense” the knowledge implemented in ASTEC, and through ASTEC, the knowledge acquired from dedicated experiment, so
they represent also a practical way to use this knowledge in other codes (like the deterministic PSA 2 tool) or to communicate this knowledge to partners interested by a condensate of the experiment.

- Bayesian network methods: basically they are designed to represent probabilistic relationship between uncertain input variables and output variables of the code. Built on the basis of numerical experiments, they allow the prognostic as well as the diagnostic of accidental sequences, knowing few observations of the scenario. They are by nature particularly relevant and useful for crisis management purpose.

Although these methods are already available and, even more, already used on the basis of ASTEC calculation, the aim in ASTEC+ is to promote such approaches and to offer generic tools to facilitate such applications. Due to the huge number of calculations they necessitate to be generated, the promotion of such methods implies promoting a high level of performance and robustness of code as well.

7. CONCLUSIONS

ASTEC V2.1 has reached a good level of performance in terms of models availability, numerical performance, robustness and reliability which authorizes its full application in current nuclear safety studies. For instance,

- ASTEC V2.1 is intensively used at IRSN for the assessment of EDF proposal of modification on their plant fleet;
- ASTEC V2.1 is also currently applied with the objective of the re-assessment of the source term relative to nuclear plants;
- The different benchmarks performed in the framework of BSAF and crosswalk exercise concluded to reasonable confidence in the whole degradation phenomena but highlighting discrepancies hardly resolved today by available experimental knowledge;
- ASTEC benefits from the expertise and the knowledge of the most important contributors to Research and Development in the Severe Accident phenomena reinforced though the NUGENIA collaborative platform within the ASCOM project.

This version will be maintained and developed in some extend for the next five years at least in order to perform the simulations of severe accident in nuclear power plant needed by our internal and external users.

In parallel, important needs motivated an inflexion of ASTEC scheme of development:

- The need to enlarge significantly the scope of use of ASTEC to deal with new facilities, new configurations in currently modeled facility;
- The need to review in depth some assumptions of the models implemented in ASTEC;
- The need to enlarge the scope of application of ASTEC models, beyond the horizon of the integral system code;
- The need to benefit from experienced methodologies of development aimed gaining at in flexibility, compactness, robustness and performance.

This inflexion will be implemented by a new trajectory of development, the so-called ASTEC+ pathway:
• Adressing severe accident phenomena whatever the nuclear facility and the context of use;
• Promoting multi-scale approaches as well as advanced algorithms;
• Ensuring the compatibility with current series of ASTEC version whereas developing new application in C++ language based on the solid roots of experienced oriented object numerical platform.

NOMENCLATURE
ASCOM: AStec COMmunity project
ASTEC: Accident Source Term Evaluation Code
BSAF: Benchmark Study of the Accident at the Fukushima Daiichi Nuclear Power Station
CEA: Commissariat à l’Énergie Atomique
EDF: Electricité De France
EPR: European Pressurized Reactor
ERVC: External Reactor Vessel Cooling
FP: Fissions Products
IRSN: Institut de Radioprotection et de Sûreté Nucléaire
ISTP : International Source Term Program
IVMR: In-Vessel Melt Retention
IVR: In-Vessel Retention
MAAP: Modular Accident Analysis Program
MCCI: Molten Corium Concrete Interaction
MELCOR: Methods for Estimation of Leakages and Consequences of Releases
NPP: Nuclear Power Plant
NUGENIA: NUclear GENeration II & III Association
OECD: Organisation for Economic Co-operation and Development
PSA2: Probabilistic Safety Analysis of level 2
RCS: Reactor Cooling Circuit
SA code: Severe Accident code
SNL: Sandia National Laboratories
STEM: Source Term Evaluation and Mitigation program
TEPCO: Tokyo Electric Power Company
TOLBIAC-ICB: Code developed by CEA to address MCCI phenomena
TMI-2: Three Mile Island Unit 2
US-NRC: US U.S. Nuclear Regulatory Commission

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