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APPENDIX 16A - COMPUTER CODES USED IN CHAPTER 16

This appendix briefly presents the computer codes used for RRC-B analyses. Since RRC-A analyses use the same codes as for design basis analyses, i.e. CATHARE, MANTA, SMART, FLICA and CONPATE, the reader is referred to Appendix 14A, "Computer Codes used in Chapter 14", which describes these codes.

The following table lists the codes which are used for the analysis of severe accidents, their current field of application and in which sub-section of Sub-chapter 16.2 these codes are used.

Appendix 16A section	Code	Application	Used in PCSR sub-section(s)
16A.1	MAAP	• Analysis of primary system response, including the prediction of mass, energy and fission product releases into the containment • Analysis of the efficiency of the primary depressurisation	• 2.1 of Sub-chapter 16.2 In-vessel accident progression and selection of relevant scenarios • 2.2 of Sub-chapter 16.2 Assessment of primary system depressurisation
16A.2	COCOSYS	• Analysis of containment pressure and temperature • Fission product transport in the containment and source term to the environment	• 2.5 of Sub-chapter 16.2 Containment pressure and temperature • 3.0 of Sub-chapter 16.2 Radiological consequences of core-melt sequences
16A.3	COSACO	• Analysis of molten core concrete interactions in the reactor pit and core catcher	• 2.4 of Sub-chapter 16.2 Assessment of melt stabilisation
16A.4	WALTER	• Calculation of time-dependent 1D-temperature profiles within the melt, protective layer and basemat	• 2.4 of Sub-chapter 16.2 Assessment of melt stabilisation
16A.5	CORFLOW	• Analysis of melt spreading	• 2.4 of Sub-chapter 16.2 Assessment of melt stabilisation
16A.6	CHEMSAGE	• Fission product release from molten pools	• 3.0 of Sub-chapter 16.2 Radiological consequences of core-melt sequences
16A.7	GASFLOW	• Analysis of hydrogen distribution and laminar combustion	• 2.3 of Sub-chapter 16.2 Assessment of hydrogen control
16A.8	COM3D	• Analysis of flame acceleration processes and fast deflagration	• 2.3 of Sub-chapter 16.2 Assessment of hydrogen control
16A.9	PAREO 9	• Analysis of containment pressure and temperature in design basis accidents	• 1 of Sub-chapter 6.2 Containment function requirements and functional design

These codes have undergone validation and verification, which is to compare and to examine the code response with the results of experiments representative of the respective conditions expected in the reactor case as well as benchmarking with other codes. This is a continuous process as is the resulting improvement of the codes.

Given an adequate outcome of the validation and verification process, the codes are considered suited to extrapolate the results of the representative tests analysed to reactor scale. Following this approach, the experimental basis largely contributes to making the severe accident mitigation strategy plausible.

Therefore, this appendix does not only constitute a mere description of codes, but is also concerned with the respective validation and verification basis.

A more detailed description [Ref-1] of the chemical aspects of the models used in these codes is available.

1. MAAP 4

The Modular Accident Analysis Program (MAAP) version 4 [Ref-1] to [Ref-5] is a computer code that can simulate the response of light water reactor power plants during severe accident sequences, including actions taken as part of accident management. The code can simulate both current designs and Advanced Light Water Reactors (ALWRs) and there are two parallel versions, one for boiling water reactors and one for pressurised water reactors. The code can be used for Level 1 analyses to determine whether a given specification of initiating events and recovery times leads to core damage and/or recovery. It can also be used in Level 2 analyses to determine containment response and fission product release histories to the environment.

MAAP4 is categorised as an "integral severe accident analysis tool" which means that it integrates a large number of phenomena into a single plant simulation (NSSS + containment + auxiliary building) such as

- thermal-hydraulics,
- core heat up and melt progression,
- lower plenum debris behaviour,
- thermal and mechanical responses of the Reactor Pressure Vessel (RPV) lower head,
- hydrogen production, transport and possible combustion,
- direct containment heating (DCH),
- molten core concrete interaction (MCCI), and
- fission product release, transport and deposition.

A dedicated report presents a detailed description of in-vessel physical and chemical models (phenomena listed above) used in the MAAP4 code and its validation [Ref-6]. A specific study [Ref-7] presents the MAAP4 modelling of corium behaviour in the RPV bottom head, RPV failure mechanisms, and conditions of corium discharge from the vessel to the reactor pit.

Models are included for engineered safeguard system logic and performance. Also, operator actions are simulated by specification of intervention conditions and responses.

MAAP was originally developed during the Industry Degraded Core Rulemaking (IDCOR) program in the early 1980's by Fauske & Associates, Inc. (FAI). It is now the property of the Electric Power Research Institute (EPRI) and is licensed by EPRI to utilities and other organisations. MAAP4 development has been partially supported by the U.S. Department of Energy Advanced Reactor Severe Accident Program.

The accident analysis of RRC-B sequences has been performed with the French 4.04 version of MAAP4. This version, which contains specific models such as that for the heavy reflector, is used as a reference code for in-vessel severe accident deterministic analyses in the context of the EPR project. In addition, code results concerning mass and energy release, fission products, hydrogen production, with and without in vessel reflooding, and corium releases from the vessel are utilised as input for containment codes used for the determination of source terms. PSA Level 2 analyses are also performed with MAAP4 where both in-vessel and results concerning the containment response are used.

MAAP has been benchmarked against a wide range of separate effects experiments and integral experiments, including actual industry experience (TMI-2 in particular). This benchmarking effort performed by the code developers/suppliers (FAI/EPRI) addresses most of the physical processes that are described by MAAP [Ref-1]

2. COCOSYS

The containment code COCOSYS (Containment Code System) [Ref-1] is a lumped-parameter multi-compartment code developed by Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) mbH for best estimate analyses of the containment behaviour in severe accidents including fission product release to the environment. To this end, the code includes models for all relevant severe accident processes and phenomena, such as containment thermal-hydraulics, and aerosol and fission product behaviour. These models address both transient processes, which mainly occur early in the accident, and slow processes, which mostly concern the long-term phase of a severe accident. Due to the large spectrum of available models and the flexibility of nodalisation schemes available, the code can be used for many tasks in the analysis of containment response.

The complete code system COCOSYS consists of several modules, which address different phenomena:

- The THY main thermal hydraulic module describes the thermal hydraulics inside the containment, e.g. gas distribution, pressure build up, hydrogen combustion, and behaviour of safety systems. The thermal hydraulic model contains a thermodynamic non-equilibrium model based on the RALOC Mod4 code version [Ref-2] [Ref-3].

- The AFP aerosol fission product module contains models for aerosol and fission product behaviour based on the aerosol and fission product part of FIPLOC [Ref-4], which derives from the MAEROS code (aerosols) [Ref-5] and the IMPAIR code (iodine) [Ref-6] [Ref-7]. The MCCI module CCI is based on the WECHSL [Ref-8] program. Extensions to the chemical data base have been added using the CHEMAPP library tool [Ref-9]. However, the CCI module of COCOSYS is not used in the analyses, since the MCCI code COSACO is employed for the analysis of the MCCI in the reactor pit and spreading compartment of the EPR.

The modules are coupled via the software PVM (Parallel Virtual Machine) [Ref-1], which ensures the full modularity of the whole code system. In addition, simplified and detailed hydrogen recombiner models, a pyrolysis model and fission product transport models including radioactive decay are available. Specific phenomena such as aerosol transport to sumps by draining wall condensate and the impact of a spray system on thermodynamics and aerosol behaviour are also modelled.

COCOSYS is specifically suited to model fission product transport in the containment and other buildings, in particular because of its

- flexible modelling of the plant buildings and technical systems including release paths,
- state-of-the-art modelling of aerosol behaviour (including hygroscopic effects and steam condensation),
- options to track decay chains and transport of radionuclides and to consider their decay heat release using the FIPHOST [Ref-10] and FIPISO [Ref-11] modules,
- state-of-the-art iodine behaviour based on the IMPAIR code with improved data set.

The code has been extensively validated [Ref-12] to [Ref-14] on several experiments (including sensitivity studies): ACE (L6), ACE-RTF (3B), AHMED, BETA (V5.1), BMC (F2, HYJET 4, Gx4, VANAM-M3), BNWL, DEMONA, HDR (E11.4, T31.5, E11.8.1), GKSS (M1), KAEVER, LACE, NUPEC (B-8-3, B-9-4, M7.1), PANDA (BC4, PC1, ISP42), PHEBUS-FP and ThAI.

3. COSACO

The philosophy behind the modelling approach followed in COSACO [Ref-1] is to produce a coherent description of the thermo-chemical behaviour and heat transfer characteristics of the oxidic melt.

Specifically, the heat transfer modelling of the oxidic melt obeys the relevant characteristics of solidification of multi-component melts as observed in industrial applications, e.g. moulding. Accordingly, the melt is modelled in such a way that it predominantly solidifies and deposits as a crust at the cold boundaries of the pool. Crust formation commences during the incipient phase of the MCCI after the melt temperature falls below the liquidus temperature curve.

On the other hand, MCCI exhibits a unique phenomenon which is not seen in moulding; the continuous mixing of the melt pool with relatively cold concrete decomposition products. As a result, solidification also takes place in the volume away from crust formation at the boundaries of the melt pool. This phenomenon is addressed in COSACO. Correspondingly, solid phases are also modelled as staying in the melt volume where they increase the viscosity and thus lead to a reduction in the heat transfer rate at the melt/crust interface.

Eventually, the combination of crust-limited heat removal and the effect of increasing viscosity results in a severe limitation of heat removal out of the melt pool which is already at a high temperature.

Contrary to the way that oxide melts are modelled, the heat transfer model developed for metallic melts is based on the assumption that a slag layer formed at the melt/concrete interface limits heat removal from the melt rather than the melt itself.

The specific modelling of thermo-chemical phenomena in the multi-component melts under consideration addresses the behaviour established in real solutions (as opposed to ideal solutions). To this end, the real solution database COSCHEM is integrated into the modelling logic of COSACO which also employs the equilibrium solver CHEMAPP [Ref-2]. The data in COSCHEM are essentially based on the real solution database TDBCR 99 [Ref-3], which was developed and validated in the CIT project of the EU's fourth framework programme.

This approach provides a consistent thermo-chemical state of the melt for non-idealised conditions involving all relevant melt components to be determined. Accordingly, complex chemical reactions become predictable concurrently with phase transitions following a change of state.

The modelling of the melt pool configuration takes two situations into account. In the case of a stratified configuration, phases having an oxidic character either concentrate in an oxidic or in a slag layer, while the metallic phases accumulate in a metallic layer. These thermo-chemically immiscible layers are connected by mass and energy transfer. Alternatively, a mixed model has been developed to study the consequences of postulated gas-induced mechanical mixing on temporary melt retention.

The cavity model is two-dimensional to allow the prediction of ablation front progression in downward and radial directions.

COSACO has been validated [Ref-4] against representative large-scale experiments either involving prototypic oxidic or metallic melts. In terms of the oxidic melts, the code was validated against the MACE tests M3b and M4 [Ref-5] [Ref-6], ACE 5 [Ref-7], OECD-CCI-1 [Ref-8] and, most recently, OECD-CCI-2 [Ref-9]. With respect to metallic melts, the code was validated against 2D-transient, large-scale tests conducted in the frame of the German CORESA project [Ref-10] to [Ref-12] as well as the SURC4 [Ref-13] and the BETA 5.2 [Ref-14] tests.

The physical and chemical models used in the analysis are detailed in a dedicated report [Ref-15].

4. WALTER

The code WALTER (Wall Temperature) [Ref-1] is used for the calculation of time-dependent one-dimensional temperature profiles within the melt, protective layer and basemat.

The code solves the Laplace equation for linear, cylindrical and spherical geometry using an speed-optimised implicit numerical scheme. It can model any number of different material layers, nodes and gaps. Other features are:

- non-uniform mesh size,
- allowance for volumetric expansion (time-variable mesh size),
- phase changes, simultaneous freezing and melting of multiple regions,
- temperature dependent properties (e.g. conductivity, viscosity),
- pressure dependent boiling curve or radiation at the surfaces,
- gaps with convective and/or radiation-dominated heat transfer,

- time dependent volumetric heat.

For the material properties and heat-transfer coefficients an explicit method is employed, as they are calculated on the basis of the temperatures of the preceding time-step.

A specific feature of the code is the consideration of horizontal molten regions. These regions are included in the implicit numerical scheme by the use of effective thermal conductivities. As convection and conduction are based on different physical mechanisms, the calculated temperature fields within the liquid layer are only rough estimations. However, the models ensure realistic heat fluxes and temperatures at the boundary of the liquid region.

The general procedure is as follows. Prior to every time-step all nodes are scanned to determine whether their temperatures exceed the liquefaction temperature of the corresponding material. For single-phase fluids this temperature corresponds to the melting temperature of the material, and for two-phase mixtures to the temperature associated with an input-specified solid fraction. Adjacent molten layers consisting of different materials are handled separately, but mixed if they consist of the same material.

Based on the spatial extent of each liquid region as determined in this first step, the relevant boundary temperatures are determined, and the effective thermal conductivities for all nodes within the liquid region are calculated using models that represent the specific physical situation.

To simulate the spread melt in the EPR, the model proposed by Baker, Faw and Kulacki for a one-dimensional, volumetrically heated, liquid pool, cooled at either bottom and/or top [Ref-2] is used. To be applicable to oxidic corium melts with temperature-dependent properties, a representative, average layer temperature is internally calculated using either all temperatures in the liquid region or an average of boundary layer and bulk temperature.

5. CORFLOW

CORFLOW [Ref-1] [Ref-2] simulates the free surface flow of a single-component, homogeneous fluid in a three-dimensional, plane or cylindrical geometry (with the optional covering of the fluid by an isothermal ideal fluid). In addition to the fluid, several structural materials can be considered as hydrodynamic obstacles or thermodynamic heat structures. The fluid is assumed to be incompressible and Newtonian.

The fluid dynamics is described by the continuity equation and the Navier-Stokes equations using the Boussinesq approximation. Volume expansion is neglected and turbulence models are not employed. Rigid boundaries are modelled as impenetrable without slip. A free surface pressure boundary condition includes viscous stress and surface tension effects. The free surface is assumed to be representable by a single valued function. For the calculation of the surface dynamics, an equation is utilised which results from the kinematic free surface boundary and the integration of the continuity equation in the vertical direction.

The hydrodynamic process of fluid flow is coupled to the thermodynamics because of the strong temperature dependence of the rheology. For this reason, internal heat transfer (by conduction and convection) and heat generation (e.g. by radioactivity) as well as heat transfer to the surroundings are modelled. At the rigid boundaries, heat transfer by conduction is assumed, whereas heat transfer by convection and radiation is modelled at the free surface. All the material properties except surface tension (i.e. density, viscosity, heat conductivity and specific heat), depend on temperature.

A discrete phase transition model is available to simulate solidification and melting of the homogeneous fluid and phase transitions of the structural materials, for example. Complex rheology and the mechanical stability of crusts are not considered. A two-phase flow model is used to describe the mushy region of the phase diagram, where the solid phase is assumed to be dispersed in the liquid phase. Below the liquidus temperature, this leads to fluid immobilisation caused by an increase of viscosity for the mushy fluid. Chemical interactions are not simulated.

The mathematical model is based on solving the continuity, Navier-Stokes, free-surface and heat equations in an Eulerian formulation. The finite volume method employs a rectangular, curvilinear, staggered grid, with not necessarily uniform cell widths. The numerical representation includes implicit difference schemes for the Navier-Stokes and free-surface equations and an explicit finite difference scheme for the heat equation. A Poisson equation for the pressure is derived from the continuity and Navier-Stokes equations, which is solved by a Chebyshev method and leads to a velocity-pressure iteration. Two representations of the free surface location are used: a second-order polynomial or a step profile.

6. CHEMSAGE AND GEMINI

The thermo-chemical programs CHEMSAGE [Ref-1] and GEMINI [Ref-2] are Gibbs energy minimisers, which in combination with an appropriate thermo-chemical database calculate complex chemical equilibria in multi-phase, multi-component systems. Such systems can consist of up to 30 chemical elements forming up to 1100 chemical compounds. In relation to nuclear reactor safety, the codes are used to compute the core melt constitution, chemical reactions within the core melt, the distribution of core melt components between different core melt fractions, and the fission product distribution between gaseous and condensed phases of the core melt in order to predict the release of fission products. Different core melt fractions can be modelled as mixture phases (e.g. oxidic melt and metallic melt). Mixture phases can be considered as ideal solutions (simplified case) or as non-ideal solutions (real solutions) depending on the thermo-chemical database that is used. Various thermo-chemical models are contained in the codes and used to model real solution thermo-chemistry.

In the context of the EPR, the codes are used to predict fission product behaviour during the ex-vessel stage of a severe accident and, in particular, the releases from MCCI pools.

7. GASFLOW

7.1. PROGRAM CHARACTERISTICS

GASFLOW [Ref-1] is a best-estimate finite-volume computer code developed at Los Alamos National Laboratory in USA and Forschungszentrum Karlsruhe (FZK) in Germany for predicting the transport of steam/hydrogen/air mixtures as well as the recombination and combustion of hydrogen. It also has the possibility of adding other gases for simulating design basis or severe accidents in the containment of nuclear power plant.

The prediction of the mixture quality is achieved by solving the transient, three-dimensional, compressible continuity, Navier-Stokes and energy equations for multi-component gas mixtures.

GASFLOW solves these transport equations in Cartesian or cylindrical co-ordinates for a multiple component gas mixture using algebraic or k-ε turbulence models as desired.

Heat conduction within walls and structures is one-dimensional and takes into account the steam condensation and film evaporation at the surface of the structures and on sump surfaces.

A one step chemical kinetics model with an Arrhenius formulation is applied to describe the chemical reaction of hydrogen with oxygen during the deflagration process.

Based on the knowledge of the recent EPRI/EDF test results [Ref-2] the recombiner models have been extended (compared to the model used during basic design) to take into account both low oxygen and low hydrogen concentrations.

7.2. MAIN FEATURES

As usual for CFD-codes, the entire control volume is subdivided in computational cells with 6 cell faces, which are connected with each other at the cell faces. Each cell has an atmosphere with homogeneous gas composition and one equilibrium temperature for all the gas components. The transport and mixing of the gas component are modelled by solving Navier-Stokes equations taking into account the conservation of each gas component. Mass and energy transport can occur to and from the structure surfaces using heat and mass transfer laws.

GASFLOW predicts the following phenomena in the course of an accident:

- pressure and temperature,
- distribution of the gases in the containment,
- stratification of the gases in the containment,
- removal (recombination and burning) of burnable gases (H_2 and CO),
- heat and mass transfer to the structure,
- natural and forced convection flows,
- gas diffusion between neighbouring cells,
- distribution of decay heat (associated with noble gases),
- heating and cooling of the atmosphere,
- leakage flow to the environment,
- gas jets.

GASFLOW uses the sigma criterion [Ref-1] [Ref-2] to determine whether a given mixture composition can support fast deflagration and the 7 lambda criterion [Ref-3] [Ref-4], to determine whether DDT (deflagration to detonation transition) is possible. While the sigma criterion is evaluated locally, the lambda criterion also takes into account the size of the gas cloud in terms of the characteristic length lambda.

GASFLOW allows a fine nodalisation (of the order of a hundred thousand cells) of a complex three-dimensional geometry without excessive requirement for computer time. This enables the code to calculate the gas distribution in the containment in detail over a long-term transient.

Mainly to take into account the requirements for long-term containment analyses, GASFLOW has been improved in the past years by adding

- a thermal radiation model to better predict pressurisation and wall temperatures,
- a simplified sump model (only one sump) to gather all condensate, and
- a spray model.

In the basic version of GASFLOW, no explicit models for a spray system existed. Instead, the classical two-phase homogeneous equilibrium model was solved with the assumption that liquid droplets were dispersed in a gaseous medium. This meant that thermal and mechanical equilibrium (equal temperatures and velocities) always existed between the phases. In order to improve this situation for GASFLOW, FZK has developed a simplified model to treat spraying [Ref-5] based on the following assumptions:

- mechanical equilibrium between the phases (equal velocities),
- thermal non-equilibrium between the phases (non-equal temperatures).

In particular, this means:

- Droplet temperatures: A specific internal energy equation for the liquid phase is now required. The gas temperature is computed from the gas internal energy, which is obtained by subtracting the liquid droplet energy from the total energy. The liquid temperature is similarly calculated from the internal energy function for the liquid.
- Pressure: The pressure field is determined from the gaseous components only.
- Heat and mass transfer: Convective heat transfer and phase change mass transfer is possible between liquid and vapour components to obtain appropriate coupling phenomena.
- Droplet depletion: Droplet depletion, sedimentation and rainout are also modelled.

7.3. MATHEMATICAL METHOD

GASFLOW uses both Lagrangian and Eulerian methodologies. The first one describes the motion of specific elements of matter as a function of space and time. This specification reduces the artificial numerical diffusion wherever it is used. However, the second one is generally more convenient because it describes flow in terms of volumes fixed in space (computational cells).

The three-dimensional, compressible Navier-Stokes equations and the conservation equations for each gas component are integrated using the Los Alamos ICE'd-ALE (Implicit Continuous-Fluid Eulerian; Arbitrary-Lagrangian-Eulerian) [Ref-1] [Ref-2], numerical methodology. Both thermal and caloric equations of state complete the equation system, which describe the respective relations between pressure, density, temperature, concentration of the gas components, internal energy and specific heat.

7.4. DOCUMENTATION, VALIDATION AND EXPERIENCE

GASFLOW is documented by four code manuals [Ref-1], which describe the governing physical equations and the computational model (Theory and Computational Model Manual), the preparation of the input data (User's Manual), verification and validation calculations (Assessment Manual) and procedures for making extensions and documentation of the code (Programming Guide Manual), respectively.

The experimental facilities used to validate GASFLOW vary from small shock tubes up to the former large-scale HDR facility (the containment of a decommissioned nuclear power plant) located close to Frankfurt, Germany.

Within the HDR facility many experimental tests have been performed during recent decades. The E11.2 and E11.4 experiments can be considered as the most important experiments for hydrogen distribution and mixing. These experiments simulated high and low elevation for hydrogen and steam release. The results of these experiments showed clear stratification or homogenisation of the atmosphere depending on the release position (high or low). Post-test calculations with GASFLOW have been performed, showing rather good agreement on the hydrogen distribution [Ref-2] [Ref-3].

Apart from HDR, emphasis in the validation of GASFLOW was laid on the many Battelle experiments [Ref-4], including experiments with combustion and jet injection. Most recently experiments at the Phebus facility (FPT0) [Ref-5] and the new ThAI facility [Ref-6] are being used for validation. In the future, new facilities, which are dedicated to CFD code validation, such as the CEA facility MISTRA or the IRSN facility TOSQAN [Ref-2] [Ref-7] [Ref-8] may be used for further validation of GASFLOW.

Several experimental qualification programs have been performed for recombiners, e.g. in the IRSN facility KALI [Ref-9], with the result that the recombination rate can be well described by the model in GASFLOW.

The GASFLOW spray model has been validated based on post-calculations of TOSQAN and MISTRA experiments [Ref-10].

8. COM3D

8.1. PROGRAM CHARACTERISTICS

COM3D is a three-dimensional code for turbulent reactive flow simulation in a complex geometry [Ref-1] [Ref-2]. COM3D has a second-order-accurate compressible Navier-Stokes equation solver coupled to turbulence and chemical kinetics models. Advanced procedures are provided to facilitate grid development for the complex three-dimensional structures required for containment analysis.

COM3D calculates the combustion progress of a pre-defined gas mixture in great detail over a few seconds. It is therefore not suited to calculate the whole thermal-hydraulic history in the containment. Consequently, COM3D must be supplemented by another CFD code such as GASFLOW, which calculates the accident progression and the mixture composition as function of time and space, and thus provides the initial data for COM3D.

As input, COM3D requires:

- geometrical data of the containment (presently COM3D assumes adiabatic conditions, but it is planned to implement models for convective heat transfer to walls, which will improve code predictions in situations close to the transition between laminar and fast combustion),
- initial conditions within the containment (gas distribution, temperature distribution, pressure distribution) when ignition occurs,
- ignition location,
- locations within the containment where accurate pressure and temperature history data for post-processing are needed.

As output, COM3D delivers:

- gas composition at pre-set moments,
- temperature and pressure distribution at pre-set times,
- flame speed distribution at pre-set times,
- accurate pressure and temperature history at pre-set locations.

8.2. MAIN FEATURES

The code describes turbulent combustion for two time regimes:

- The turbulent time scale is larger than the reaction time scale (Da > 1): distributed reaction zones.
- The turbulent time scale is smaller than the reaction time scale Da < 1: well stirred reactor.

Here Da is the Damköhler number, which relates turbulence and chemical time scales [Ref-1] [Ref-2].

Two different turbulence models are available within the code:

- a standard k-ε model (used for all calculations in the PCSR) [Ref-3],
- a Renormalisation Group Theory RNG k-ε model [Ref-4].

The RNG model is a modern enhancement of the traditional k-ε model. An additional term has been added in the k-ε equation which changes dynamically with the rate of strain of the turbulent flow, thereby providing more accurate predictions for flows with large eddies.

The RNG model appears attractive for a number of reasons:

- It is applicable to compressive flow.

- The model parameters result from a closed theory, not from empirical experiment data.
- It covers low Reynolds numbers.
- Additional computational costs compared to the standard k-ε model are low (~3%).

With respect to turbulent combustion modelling the code offers:

- an eddy dissipation model and an eddy break-up model for Da > 1,
- an Arrhenius formulation for the well stirred reactor (Da < 1).

In addition, combustion modelling is extended to treat intermediate mixing states for each component with a presumed β probability density function (PDF) model. The PDF model is based on a statistical description of the reacting media. It introduces probability density functions for the model parameters such as species concentrations, temperatures, etc. This model has not been applied so far for calculations presented in the PCSR.

8.3. DOCUMENTATION, VALIDATION AND EXPERIENCES

COM3D had been validated using experiments performed at different scales with generally good agreement for important physical quantities. The validation of the code, in particular with respect to low hydrogen concentration around 11% by volume, has been performed in the framework of the EU HYCOM project [Ref-1], using also some new experiments in the large RUT facility [Ref-1] to [Ref-3] and in smaller facilities, such as TORPEDO and DRIVER [Ref-4], all at the Kurchatov Institute, Moscow.

The first type of combustion tests are medium scale experiments, which were carried out in the 12 m FZK combustion tube. The comparison of calculated against experimental data generally shows very good agreement for the acceleration phase (0 to 0.01 seconds) as well as for details of the subsequent combustion phase, including velocity and pressure values for incoming, reflected and transverse waves.

The experiments can be separated into four groups, depending on the main features of flame acceleration:

- fast acceleration leading to DDT (typical flame velocities before DDT are 1200 m/s for a test with 20% hydrogen by volume and a blockage ratio of 0.3),
- fast acceleration and then propagation in the 'sonic' regime (typical velocities are 600 to 700 m/s for a test with 15% hydrogen by volume and a blockage ratio of 0.6),
- acceleration at a moderate rate up to the end of the tube (typical velocities are 400 to 500 m/s for a test with 12% hydrogen by volume and a blockage ratio of 0.6),
- unstable regime, characterised by a short initial acceleration phase followed by local quenching with a series of possible re-ignitions (typical velocities are less than 100 m/s for a test with 10% hydrogen by volume and a blockage ratio of 0.3).

Without the PDF model, it was found that only experiments of the first three types could be simulated successfully, while the experiments with local quenching appeared to be not reproducible with the adopted combustion model. However, it was found that the present modified eddy break-up model provides conservative results with respect to flame velocity and thus also to pressure loads.

The modified eddy break-up model produces satisfactory results in the following ranges: $10^2 < Re < 10^6$ and $12.5 < Da < 1250$. Here Re is the Reynolds number. This domain covers almost the whole region of interest in industrial applications, excluding the relatively narrow part of thickened flames where $1 < Da < 10$, and therefore provides a good basis for numerical simulations of the processes.

To complement the tests in the FZK tubes, a second type of tests consisting of large-scale experiments on hydrogen-air and hydrogen-air-steam combustion have been performed, in particular at the Kurchatov Institute in Moscow in the framework of several EU projects such as HYCOM [Ref-1].

Turbulence modelling was tested in a shock tube model of the 12 m tube. In this model, the tube was divided by a membrane into a low-pressure section (length 9 m) containing circular orifices as obstacles and a high-pressure section (length 3 m). After evacuating both sections, the low-pressure section was filled up to the initial pressure of 1 bar by air. The high-pressure section was filled with helium until the membrane burst. After bursting of the membrane a shock wave travels into the remaining section. The measured pressure signals at different locations can then be compared with the numerical simulations using different turbulence models. The advantage is the validation of turbulence models separately from combustion.

As already mentioned, in some HYCOM experiments, in particular in an experiment performed in the DRIVER facility, the conservatism of COM3D for lean hydrogen/air mixtures has been demonstrated. In this experiment the tube had been subdivided by a membrane into two parts. In the first part, which was filled with 13% hydrogen by volume and then ignited, flame acceleration was calculated with COM3D up to 800 m/s (compared to the measured value of 600 m/s and predictions of 600 to 1000 m/s by other codes). In the second part of the tube, which was filled with 10% hydrogen by volume, a significant deceleration of the flame down to 200 m/s was found in the experiment. The flame velocity calculated with COM3D stayed constant at 800 m/s, which clearly demonstrated the conservatism of the code for lean mixtures [Ref-5].

9. PAREO

9.1. GENERAL PRESENTATION OF PAREO 9

PAREO [Ref-1] was developed by EDF-SEPTEN to determine pressure and temperature changes within the containment of a pressurised water reactor (or any other leak-free enclosure) after the accidental release of water or water vapour following a pipe break (primary or secondary coolant or other system).

The studies normally conducted with PAREO have two main objectives:

- to determine the value of the pressure peak in the containment by calculation of the first few minutes of the accident (severe accident, LOCA, surge line break, steam line break),

- to determine the long-term changes in the containment pressure and the temperature of the atmosphere, water and structures in the event of a LOCA or a severe accident, in order to check the design validity in the RRI [CCWS] or RRI [CCWS]/SEC [ESWS] heat exchangers making up the residual heat removal system, and the strength of the structures with reference to the cumulative pressure and temperature stresses.

To this end, various systems in the containment are represented, along with their interactions, as are different models:

- gaseous phase,
- liquid phase,
- materials liable to absorb or output heat,
- the containment heat removal system (EVU [CHRS]), the safety injection system (RIS [SIS]) and the EVU [CHRS]/RRI [CCWS]/SEC [ESWS] heat exchanger systems,
- modelling of conduction in the structures processed by an independent calculation module (COMOD),
- differentiation between the air components and the possibility of combustion of the hydrogen,
- modelling of various hypotheses for separation of the two-phase mixture released at the breach into a vapour phase and a liquid phase,
- incorporation of water vapour condensation on cold walls,
- incorporation of water vapour condensation on spray droplets.

Code data consists of:

- the geometry of the containment and the materials it contains (free volume, thickness of concrete, steel, exchange surfaces, etc.),
- the initial conditions (temperature, pressure, etc.),
- data concerning the cooling systems (spray, injection, exchangers, etc.),
- the masses and energies released at the breach.

The code outputs the evolution of the following values as a function of time:

- temperature and pressure in the gaseous and liquid phases,
- temperatures within the heat conduction systems,
- temperatures of cooling fluids (EVU [CHRS], RRI [CCWS], SEC [ESWS]),
- values for the various mass and energy transfers.

In the most common application of PAREO, concerning the design of pressurised water reactor containments, the choice of parameters and hypotheses is made in order to maximise the value of the pressure peak. The hypotheses can be said to be conservative with respect to the pressure peak.

This conservative approach consists of increasing and accelerating the mass and energy inputs to the containment and reducing or delaying cooling (heat transfer in the structures, spraying, etc.).

9.2. MODELLING

9.2.1. Systems Modelled in the Containment

Thermal-hydraulic systems

Two thermal-hydraulic systems are modelled: one gaseous phase and one liquid phase.

- Gaseous phase:
  - The gaseous atmosphere consists of a mixture of air, water vapour and possibly hydrogen, assumed to be an ideal gas mixture with uniform temperature and pressure throughout the volume.
  - It is assumed that the gases, except for water vapour, are perfect gases.
  - This gaseous phase exchanges mass and energy with the liquid phase and energy with the structures.
- Liquid phase:
  - This consists of water contained in the sumps at the bottom of the containment and exchanges mass and energy with the gaseous phase and energy with the structures. Its temperature and pressure are assumed to be uniform throughout the volume.

Heat conduction systems

This includes all the materials contained in the containment, which are initially cold and liable to exchange heat with the gaseous or liquid phases. These systems can be flat or cylindrical and comprise layers of different types. Conduction inside each system is calculated one-dimensionally by a breakdown of the layers into a certain number of nodes.

A specialised module called COMOD calculates the temperatures of each node. The interface with the PAREO code is via formulas giving the heat flux exchanged with each side of the conduction systems.

Exchanges of mass end energy with the gaseous and liquid phases from other systems

- Breach:
  - The release point (breach) can be located on the primary system, the secondary system or any other system liable to release mass and energy into the containment.

- Containment heat removal system (EVU [CHRS]):
    - In the case of a severe accident (RRC-B or RRC-A events), the system is capable of transferring the residual heat from the IRWST to the ultimate heat sink via an intermediate cooling system (RRI [CCWS] - SEC [ESWS]) which cools the water of IRWST via a heat exchanger.
    - In such a case the system is also capable of transferring the residual heat from the containment atmosphere to the IRWST in order to control the containment pressure by spraying into the dome area. The condensate flows back to the IRWST, is cooled by the heat exchanger and then routed back to the spray nozzles.
- Safety injection system (RIS [SIS]):
    - This system is characterised by the flow rate and temperature of the water in the system and by the characteristics of the exchanger in the recirculation phase.
- Cooling systems in recirculation phase:
    - During this phase of the accident, the spray and injection water is taken from the sump and can be cooled either by raw water (SEC [ESWS] system) or via the component cooling system (RRI [CCWS]).
    - These cooling systems are characterised by their exchange coefficients, the exchange surface of the various heat exchangers, the water flow rates through these exchangers and the raw water temperature.
- Containment cooling:
    - The code can take account of possible cooling of the containment (cooling coils, etc.).
- External medium:
    - The external air and the ground exchange energy on contact with certain heat conduction systems (containment, raft, etc.).
- Hot structures:
    - Another feature offered by the code is calculation of the energy given off by hot structures.

9.2.2. Mass and Energy Exchanges between the Various Systems

It is assumed that all heat and mass transfers are instantaneous, in other words, in a given time step, mass and energy pass directly from one system to the other. Similarly, any state changes are instantaneous (no delay in condensation, boiling, etc.).

Hypothesis concerning water released at the breach

Two hypotheses are used in the code:

- Total mixing of the fluid released at the breach with the gaseous phase.
- Separation of the fluid released from the breach into a gaseous part mixing with the containment atmosphere and a liquid part going to the sumps. This separation is assumed to take place at the total pressure prevailing in the containment. This hypothesis is known as the pressure flash method.

  This is used for the design calculations corresponding to major primary breaches. It was confirmed as being the most conservative [Ref-1].

Heat exchange between atmosphere and walls

Several types of exchange are modelled in the code:

- Exchanges by natural convection:
  - This type of exchange occurs when the wall temperature is higher than the dew point of the atmosphere.
- Exchanges by natural convection and condensation:
  - When the wall temperature is lower than the dew point of the air-water vapour mix, condensation takes place on the wall. The correlation used to describe this type of exchange is the Tagami or Uchida correlation [Ref-2].

It is assumed that part of the power absorbed by the walls comes from condensation of water vapour on the wall and that the rest comes from natural convection exchange between the atmosphere and the walls.

Heat exchange between atmosphere and spray water

When leaving the spray heads, the spray droplets are at a temperature lower than the dew point of the atmosphere. They heat up as they fall owing to convection and conduction on the one hand and to condensation of the water vapour in the atmosphere on the other, until they reach the dew point of the air-water vapour mixture. As long as there is condensation on the droplets, the physical phenomena involved are the same as for atmosphere-wall exchanges. The percentage adopted to define the relative importance of condensation and convection is identical to that chosen for exchanges with the walls.

Furthermore, to minimise the energy absorbed by the spray droplets, their final temperature is considered to be equal to the dew point of the atmosphere.

Direct exchange between sump water and atmosphere

The following is taken into account:

- condensation of the water vapour contained in the atmosphere when it is saturated,
- convection between liquid and gaseous phases,
- evaporation of sump water.

9.3. DOCUMENTATION AND VALIDATION

The PAREO 8 code has been validated by comparisons with BATELLE and CVTR experiments [Ref-1]. PAREO 9 contains the same modelling [Ref-2] and gives the same results as PAREO 8 for representative transients [Ref-3].

APPENDIX 16A – REFERENCES

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