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DÉPARTEMENT DE MODÉLISATION DES SYSTÈMES ET STRUCTURES
SERVICE DE THERMO-HYDRAULIQUE ET DE MÉCANIQUE DES FLUIDES

LABORATOIRE DE MODELISATION ET SIMULATION A L'ECHELLE SYSTEME

CATHARE

CATHARE 2 V2.5_3mod2.1 : MAIN NEW FEATURES AND IMPROVEMENTS

CSSI

DEN/DANS/DM2S/STMF/LMES/RT/12-042/A *Décembre 2012*

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Rapport technique DEN

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CATHARE 2 V2.5_3mod2.1 : MAIN NEW FEATURES AND IMPROVEMENTS

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MOTS CLEFS

CATHARE V2.5_3, INPUT DECK; FEATURES

RESUME / CONCLUSIONS

L'objectif de ce document est de décrire la version V2.5_3 de CATHARE 2 et de comparer cette nouvelle version avec la dernière version livrée. Ce document donne les nouvelles fonctionnalités de la version CATHARE 2 V2.5_3 et les principales modifications par rapport à la précédente CATHARE 2 V2.5_2. L'objectif de ce document est aussi d'aider les utilisateurs à migrer leurs jeux de données vers la nouvelle version CATHARE 2 V2.5_3.

ABSTRACT :
The purpose of this document is to describe the CATHARE 2 V2.5_3 version and to compare this new version with the latest industrial version (V2.5_2). This document gives the new features and functionalities of the CATHARE 2 V2.5_3 version and the main modifications compared to the previous one CATHARE 2 V2.5_2. The goal of the document is also to help an experienced CATHARE user to migrate his existing V2.5_2 input decks into their equivalent form suitable with the new V2.5_3 version.

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1 INTRODUCTION

The purpose of this document is to describe the **CATHARE** 2 V2.5_3 version and to compare this new version with the latest industrial version (V2.5_2).

The first chapter (NEW FEATURES IN THE CATHARE 2 V2.5_3 VERSION) of this document gives the new features and functionalities of the **CATHARE** 2 V2.5_3 version and the second chapter (MAIN MODIFICATIONS IN THE CATHARE 2 V2.5_3 VERSION gives the main modifications compared to the previous one **CATHARE** 2 V2.5_2.

By this document, the goal is also to help an experienced **CATHARE** user to migrate his existing V2.5_2 input decks into their equivalent form suitable with the new V2.5_3 version :

1. the detailed description of obsolete operators, directives and options in V2.5_3 version.
2. all new features of V2.5_3.

For such a goal, the modifcations of input decks are given in the "input data deck" culumn of this following tables where :

- the "**MAND**" label refers to **mandatory modification**,
- the "**NF**" label to **new functionnality**,
- the "**NOM**" label to **new models, options or variables**.

CATHARE 2 V1.3 users willing to use the **CATHARE** 2 V2.5_3 version should refer to [9] and complete the migration process of their applications using :

1. from **CATHARE** 2 V1.5 to **CATHARE** 2 V1.5 [5],
2. from **CATHARE** 2 V1.5A to **CATHARE** 2 V1.5B [6],
3. from **CATHARE** 2 V1.5B to **CATHARE** 2 V2.5 [7],
4. from **CATHARE** 2 V2.5 to **CATHARE** 2 V2.5_1 [8],
5. from **CATHARE** 2 V2.5_1 to **CATHARE** 2 V2.5_2 [4] using the "CATHARE 2 V2.5_3 mod2.1 code : Dictionary of operators and directives[1]".

It is assumed that the delivered package has been properly installed on your computer according to the procedure presented in the CATHARE 2 V2.5_3 installation manual [2].

2 NEW FEATURES IN THE CATHARE 2 V2.5_3 VERSION

New features are functionnalities developped either in the frame of the **CATHARE** 2 V2.5_3 development (new functionalities) or in the frame of the maintenance of the industrial and frozen versions (**CATHARE** V2.5_1 and V2.5_2 for improvment of existing functionalities).

2.1 Fluid used in CATHARE

Operator, Directive	Comment	Input data deck
FLUID	Implementation of the the heavy water (DHO, option HEAVYWAT) fluid	**NOM**
FLUID	Implementation of the lead (Pb, option LEAD) and the Lead bismuth eutectic (LBE, option LEADBISM) fluids	**NOM**

Table 2.1.1: Fluid used in CATHARE

2.2 User-friendliness of the code

Operator, Directive	Comment	Input data deck
WRITE, VALUE	The LIQMASS CCV (liquid mass) is available for a CIRCUIT and a ZONE	**NOM**
WRITE, VALUE	The PRESXi CCV (partial pressure for the i^{th} non-condensible gas for the boundary condition element) is available	**NOM**
COMPONEN	The name of the PITCH option is changed to PINPITCH for the COMPONEN PINGEONA	**MAND**

Table 2.2.1: User-friendliness of the code

2.3 Physical models

Operator, Directive	Comment	Input data deck
COMPONEN	New option (PINWIRNA) to use the a specific friction correlation (REHME) applied to pin with wire (SFR applications)	NOM
COMPONEN	New option (FRICLAW) to use the user correlation for the wall friction under forced convection (SFR, Pb and LBE applications)	NOM
OPTION	New option (NUSSELT) to use a different nusselt number in the (q_{pg}) wall to gas heat flux	NOM
ACCU	New option (NOADIAB) to take into account the influence of the wall and the interface heat exchange in the gas volume	NOM
VOLUME	New option (QLEFR62) in order to modify the flashing term of the (q_{le}) interface to liquid heat flux for the **0-D** module	NOM
WRITE, VALUE	The following CCV for film condensation are available : • PQSHER : interface to liquid heat transfer (q_{le}) sensitivity parameter in case of CHEN correlation with non condensible gas (modification of SHERWOOD number) : • PPCH : wall to interface heat transfer (q_{pi}) sensitivity parameter with CHEN correlation (WALL and EXCHANGER sub-modules). • PPSHER : wall to interface heat transfer (q_{pi}) sensitivity parameter with CHEN correlation (WALL and EXCHANGER sub-modules).	NOM
WRITE, VALUE	The following CCV are available : • PQGT : droplet flow sensitivity parameter for the (q_{le}) liquid-interface heat flux. • PVBR : rising of bubbles sensitivity parameter in lower sub-volume (module **0-D** only).	NOM
WRITE, VALUE	The SHENT sensitivity parameter of limit level used for liquid (for horizontal and upward Tee) or gas (for downward Tee) entrainment calculation and phase separation is avalaible.	NOM

Table 2.3.1: Physical models

2.4 The 1-D module

Operator, Directive	Comment	Input data deck
HYDR	Implementation of an automatic calculation model for the coefficient FRIMAPE used in the IMAPE transport scheme	**NOM**

Table 2.4.1: The 1-D module

2.5 The 3-D module

Operator, Directive	Comment	Input data deck
WRITE, VALUE	NRJERROR CCV variable removed for any kind of **3-D** element. Its value is set to INF	**MAND**

Table 2.5.1: The 3-D module

2.6 The 0-D module

Operator, Directive	Comment	Input data deck
MANIFOLD	The MANIFOLD directive, used in the data block, can be applied to any volume element to model the imbalance of liquid temperatures or radio-chemical products at the volume inlets and to carry it at the volume outlets. This directive triggers an incomplete mixture model inside the specified volume	**NF**
GEOM	Implementation of the inclination sub-module for NP applications	**NF**
GEOM	New option (GAUGE) allowing the definition of **0-D** module as level function of the capacity for NP applications	**NOM**
GEOM	New option (LAW) allowing the definition of **0-D** module as level function of the volume by a law	**NOM**
GEOM	New option (L_INFLUEN) to define the influence length at the junctions : influence length used to calculate the flow distribution coefficients at junctions. By default this length is calculated by **CATHARE**. Option also activates specific distribution coefficients for SFR fluid only	**NOM**

continued on next page

Operator, Directive	Comment	Input data deck
GEOM	Implementation of a PWR accumulator model (option (PWRACC)	NOM
LEVEL	New option (CONSERVH) to kept the initialised enthalpy of the liquid phase in the lower sub-volume and to automatically calculate the non-condensible mass fraction in the upper sub-volume. Only used in **0-D** module with non condensible gas	NOM

Table 2.6.1: The 0-D module

2.7 The wall sub-module

Operator, Directive	Comment	Input data deck
EXWALINK	Model of thermal coupling by radiation between two walls of a **3-D** module	NF
WRITE, VALUE	The ZSW CCV (curvilinear coordinate of one wall axial mesh) is available for WALL sub-module only	NOM

Table 2.7.1: The wall sub-module

2.8 The fuel and plate fuel sub-module

Operator, Directive	Comment	Input data deck
Post-processing [3]	Add of specific anti-reactivities for fuel (SFR applications) • REACTCLA : Fuel cladding thermal expansion effect on reactivity (RNR application) ($) • REACTCOO : Coolant density effect on reactivity (RNR application) ($) • REACTDUC : Hexagonal duct thermal expansion effect on reactivity (RNR application) ($) • REACTFUE : Fuel pin thermal expansion effect on reactivity (RNR application) ($)	NOM

continued on next page

Operator, Directive	Comment	Input data deck
FUELPLAQ	New option (FREE) for SFR free fuel. The anti-reactivity coefficient is resulting from fuel axial thermal expansion at a given radial mesh of the fuel layer	NOM
FUELPLAQ	The contact resistance between two materials (option RESIST) can be defined by an axial profile on a given segment	NOM
FUELPLAQ	In FNR and HTR applications, the fuel enrichment and the pellet compaction rate can be given as a axial profile (options ENRICH and TAUREMP)	NOM
FUELPLAQ	In HTR applications, new option (COEFKFE, FCOEFKFA) to take into account the thermal dilatation	NOM
FUELCHAR, FUELPLAQ	Option (LININTER) to choose between a logarithmique or a linear interpolation for the calculation of the residual and non residual power	NOM
RELOC	The RELOC directive enables the fuel relocation model after cladding burst (private library)	NF
WRITE, VALUE	The following variables are available for the FUEL relocation model (RELOC) : • RELOCDGA : diameter of fuel fragments used to calculate the residual gap. • RELOCDCO : diameter of fuel fragments used to calculate the equivalent thermal conductivity. • RELOCTXO : volume fraction of balloon filled by fuel after relocation. • RELOCGAP : gap calculated by relocation model and imposed after the cladding burst at the rupture location. • RELOCPWR : power coefficient calculated by relocation model after the cladding burst at the rupture location. • GAPCOND : conductivity in the gap. • LAMBDUO2 : UO_2 pellet conductivity. • HGAPC : conductance of gas in the gap. • FLURADI : additional external oxide heat flow.	NF

continued on next page

Operator, Directive	Comment	Input data deck
WRITE, VALUE	The following CCV for the power generated by cladding oxydation (FUEL, WALL or FUELPLAQ sub-modules) are available : • POWEROXY : power generated by cladding oxidation. • POWEROXE : power generated by cladding oxidation on external face. • POWEROXI : power generated by cladding oxidation on internal face.	NOM
WRITE, VALUE	The PXNEUT CCV (fraction of kinetic power dissipated in the fluid) is available	NOM

Table 2.8.1: The fuel and plate fuel sub-module

2.9 The reflooding sub-module

Operator, Directive	Comment	Input data deck
WRITE, VALUE	The following CCV are available for reflooding sensitivity parameters : • the rate of entrainment used in the (τ_i) interfacial friction, the (q_{le}) interface to liquid and the (q_{ge}) interface to gas heat fluxes, • the droplet diameter used in the interface to liquid (q_{le}) and gas (q_{ge}) heat fluxes, • the threshold distance used in the the (q_{pvi}) wall to interface reflooding heat flux.	NOM

Table 2.9.1: The reflooding sub-module

2.10 The flow-limiter sub-module

Operator, Directive	**Comment**	**Input data deck**
FLOW LIMITER	For a steam FLOW LIMITER, the reduced surface SR is now used for calculating the critical mass flow rate	**NOM**

Table 2.10.1: The flow-limiter sub-module

2.11 The flow-mixer sub-module

Operator, Directive	**Comment**	**Input data deck**
STARTMIX	The option DTMIX is no longer allowed	**MAND**

Table 2.11.1: The flow-mixer sub-module

2.12 Simulator use

Operator, Directive	**Comment**	**Input data deck**
OPTION	The parallel computing is available for EPR data set (ctree=EPRTH)	**NF**
MANAGE	Correction in order to enable the time management by cycles after the time specified by the user specified in MANAGE	**MAND**

Table 2.12.1: Simulator use

2.13 Coupling with others codes

Operator, Directive	**Comment**	**Input data deck**
WRITE, VALUE	Integration of tools for the coupling of **CATHARE** with other codes : • DPGEXT : pure momentum source sent to the gas phase. • DPLEXT : pure momentum source sent to the liquid phase. • OVPGEXT : indicator giving the advective term in the gas momentum equation. • OVPLEXT : indicator giving the advective term in the liquid momentum equation. • OVHGEXT : indicator giving the enthalpy considered in the convective term of the gas energy equation. • OVHLEXT : indicator giving the enthalpy considered in the convective term of the liquid energy equation. • ENTHEXT : enthalpy considered in the convective term of the gas (resp. liquid) energy equation when the OVHGEXT (resp. OVHLEXT) is < -1 or > 1.	**NOM**

Table 2.13.1: Coupling with others codes

2.14 The kinetic sub-module

Operator, Directive	**Comment**	**Input data deck**
CORE	New option (CSPLATE) to describe the core support plate conductive time constant and the anti-reactivity of core support plate (HTR applications)	**NOM**
CORE	New option (LINEARIZ) to model the boron effect on the moderator and the density anti-reactivity (PWR applications)	**NOM**

Table 2.14.1: The kinetic sub-module

2.15 Others functionnalities

Operator, Directive	Comment	Input data deck
GEOM	New option (SECTOT) to define the overall section of the jetpump (NP applications)	NOM
WALLCOM, WALLMOD and WALL	New option (NONETABLI) : a geometric factor due to transient operating conditions will be taken into account or not in the calculation of the heat transfer coefficient (for COMETE project)	NOM
BRUTEF77	The BRUTEF77 directive is used to places FORTRAN instructions provided by the user in the executable block directly into the PILOT.f subroutine (translation of the calculation scenario). This directive allows control statements during the processing, or additional steps for the scenario	NF
ASSIGN	New model for the RUPTURE module to define an external rupture (option EXTERNAL)	NF
WRITE, VALUE	The following variables are available for the **external**[1] RUPTURE submodule : • TLIQEXT : liquid temperature in the containment building. • AGEXT : void fraction in the containment building.	NF

Table 2.15.1: Others functionnalities

3 MAIN MODIFICATIONS IN THE CATHARE 2 V2.5_3 VERSION

The **CATHARE** 2 V2.5_3 version benefit from the maintenance work in the V2.5_2 version. All modifications (if applicable) include in the V2.5_2 version and particularly in the last updated V2.5_2 version (mod8.1, from update 1 to 397) have been integrated in the V2.5_3 version. The main modifications (or updates) are given in this section.

3.1 User-friendliness of the code

Operator, Directive	Comment
	Improvement of the linear interpolation with decreasing abscisses
Post-processing [3]	The maximum number of **CATHARE** evolutions for a post-processing job is increased to 500

Table 3.1.1: User-friendliness of the code

3.2 Portability of the code

Operator, Directive	Comment
	Improvment in the liquid average velocities to take into account a big step of void fraction between two adjacent meshes. Only available for the H_20 fluid
	Modification of the interface to liquid heat flux in case of liquid injection for **1-D** and **3-D** modules
	Accumulator's discharge is done only once per time step and not at each iteration (done in the frame of the modification)

Table 3.2.1: Portability of the code

3.3 Physico-numerical aspect

Operator, Directive	**Comment**
	Correction of the CCFL for **1-D** and **3-D** elements
	The traitment of the residual phases in the **3-D** elements become consistent with the **1-D** module

Table 3.3.1: Physico-numerical aspect

3.4 The 0-D module

Operator, Directive	**Comment**
	Correction of pressure calculation on the port of volumes
	Modification to take into the initial volume of the containment in the TAGAMI film condensation model
	Modification to take into account the gas void fraction in the ratio of the mass fraction of non condensible gas TAGAMI film condensation model

Table 3.4.1: The 0-D module

3.5 The 3-D module

Operator, Directive	**Comment**
	Correction to verify that the face of **3-D** on teta direction are closed. The sum of all the mesh cell lenghts on teta direction are compared to $2*pi$. An error message is introduced to avoid a sum of angles is different from $2*pi$ in the **3-D** cylindrical
	Correction of the convection schema in the momentum equation (flag IDISCRET=3). A new calculation of the Coriolis force is available
	Verification tools of porosity for **3-D** elements. Messages are redirected in the file *.porosity3D_warning
WRITE, VALUE	Correction of sensitivity parameters for the **3-D** module
WRITE, VALUE	Correction of the level location (IPOSNIV) calculation for a SENSOR in a **3-D** module

Table 3.5.1: The 3-D module

3.6 The fuel sub-modules

Operator, Directive	Comment
	Correct the maximale deformation when burst occurs on maximale rupture deformation

Table 3.6.1: The fuel sub-modules

3.7 The reflooding sub-module

Operator, Directive	Comment
	Improvement for the stop of the quench front level progression

Table 3.7.1: The reflooding sub-module

3.8 The explicit hydraulic link sub-module

Operator, Directive	Comment
EXHYLINK	Correction in order to allow the definition of an EXHYLINK between an external source and an external PIQREV
EXHYLINK	Correction of the communication between a source and a rupture element when radio-chemical components are defined
EXHYLINK	Correction of the void fraction for two linked elements. It must be greater than or equal to the minimum allowed value
EXHYLINK	Correction of the mass balance equations for two linked elements (weight of the element)
EXHYLINK	Correction concerning the link between a boundary condition and a source (or equivalent) object when radio-chemicals elements are defined
EXHYLINK	Correction of the radiochemical transfert for RUPTURE-PIQREV and BCONDIT-PIQREV links
EXHYLINK	Correction for PIQBREK-PIQREVlinks

Table 3.8.1: The explicit hydraulic link sub-module

3.9 The accumulator sub-module

Operator, Directive	Comment
ACCUMOD	Correction of the ACCUMOD directive used to change the boron concentration in the water of the accumulator

Table 3.9.1: The accumulator sub-module

3.10 The flow-mixer sub-module

Operator, Directive	Comment
FLOMIXER	Correction in case of EXCHANGER sub-module use
FLOMIXER	Correction for the radio-chemical flux distribution
FLOMIXER ZOOM	Correction of the radio-chemical flux distribution at in the outlet ports of the outgoing **0-D** module
FLOMIXER ZOOM	Correction of the reading of the mixing matrices
FLOMIXER ZOOM	Correction of the matrix normalization

Table 3.10.1: The flow-mixer sub-module

3.11 The radio-chemical sub-module

Operator, Directive	Comment
	Limitation of radio-chemical concentrations between 0 and $\frac{1}{ka}$ and creation of a radio-chemical mass error parameter

Table 3.11.1: The radio-chemical sub-module

3.12 Simulator use

Operator, Directive	Comment
PESEE	Correction of the MAILLAGE log file when using the "PESEE ON" directive

Table 3.12.1: Simulator use

3.13 SFR models

Operator, Directive	Comment
	Correction of the Pontier law for low Reynolds number (SFR applications)
	Modification of the entrainement term use in the wall friction calculation for void fraction $\alpha > 0.5$ (SFR, applications)

Table 3.13.1: SFR models

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NOTATIONS

ACRONYMS

CCFL : Counter Currant Flow Limitation. 21
CCV : **CATHARE** Computational Variables (VCC). 11–14, 16
COMETE : CATHARE application for rocket motors and engines. 19

EPR : European Pressurized Reactor. 17
FNR : Fast Neutron Reactor. 15
HTR : High Temperature Reactor. 15, 18
NP : Nuclear propulsion (navy). 13, 19
PWR : Pressurized Water Reactor. 14, 18
SFR : Sodium Cooled Fast Reactor. 12–15, 24

DHO : Heavy Water fluid. 11
H_20 : Light Water fluid. 20
LBE : Lead bismuth eutectic (LBE : eutectic alloy of lead (44.5%) and bismuth (55.5%) fluid. 11, 12
Pb : Lead fluid. 11, 12
UO_2 : Uranium pellet component. 15

END OF DOCUMENT