

Titolo

Implementation of Thermo-Physical Properties and Thermal-Hydraulic Characteristics of Lead-Bismuth Eutectic and Lead on CATHARE Code

Descrittori

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Sommario

The nuclear innovative systems cooled by Lead-Bismuth Eutectic (LBE) and pure Lead are object of an ongoing interest in Europe, but also outside, evidenced by a large number of national and international projects. Within the European Framework Programmes, hence, it has been highlighted the needs of a thermal-hydraulic system code able to treat these Heavy Liquid Metals (HLM) systems, with a particular interest for a “European” code. Taking into account this scenario a Specific Topic of Cooperation (STC) has been agreed in the frame of ENEA/CEA collaboration on Nuclear Fission with the objective of extend the capability of the French system code CATHARE to simulate HLM reactors.

The CATHARE code has been already modified in the recent past to be multi-fluid with well proven capabilities and moreover, it is already part of an European simulation platform (NURISP project) devoted to LWR system studies and aiming to be extended also to advanced reactors.

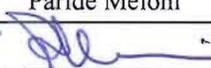
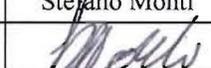
For what regards the computational phase, the implementation takes advantage of the work already done by the Cathare-Team with the properties of sodium and for what regards the material properties, thanks to the European working group WG-LBE that in the past years have collected the state-of-the-art for LBE and Lead characteristics.

This technical report summarize the work done to implement the LBE and Lead properties in CATHARE code, in collaboration/supervision with the Cathare-Team, pointing out the constraints and needs of the computational phase, the physical properties adopted, the subroutine changed and finally, some preliminary results on analytical tests.

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1. INTRODUCTION

The nuclear innovative systems cooled by Lead-Bismuth Eutectic (LBE) and pure Lead are object of an ongoing interest in Europe, but also outside, evidenced by a large number of national and international projects. Within the European Framework Programmes, hence, it has been highlighted the needs of a thermal-hydraulic system code able to treat these Heavy Liquid Metals (HLM) systems, with a particular interest for a “European” code. Taking into account this scenario a Specific Topic of Cooperation (STC) has been agreed in the frame of ENEA/CEA collaboration on Nuclear Fission with the objective of extend the capability of the French system code CATHARE to simulate HLM reactors. Furthermore, the code has been modified in the recent past to be multi-fluid [1] and it is part of an European simulation platform (NURISP project) devoted to LWR system studies but aiming to be extended also to advanced reactors.

For the ENEA has been also the opportunity to have an alternative code to the widely used RELAP5 thermal-hydraulic code to face up future commitments. The RELAP5 code, born to simulate light water reactors, was modified to treat HLM in the frame of PDS-XADS project [2] where the material properties were implemented from a semi-empirical soft-sphere model based on Monte Carlo calculation [3]. The practice in using the modified version of RELAP5 has shown some weakness in reproduce experimental data such as density and heat capacity of the coolant. So that, this physical approach based on particles interaction has not been considered viable in the case of CATHARE HLM implementation preferring to rely on experimental correlation with the possibility of future updates when new experimental evidences become available.

For what regards the computational phase, the implementation takes advantage of two keypoints: the work already done by the Cathare-Team with the properties of sodium and the thermo-physical and thermo-dynamic properties collected in an Handbook issued by OECD-NEA, that represents the state-of-the-art for LBE and Lead characteristics [4].

This technical report summarize the work done to implement the LBE and Lead properties in CATHARE code, in collaboration/supervision with the Cathare-Team, pointing out the constraints and needs of the computational phase, the physical properties adopted, the subroutine changed and finally, some preliminary results on analytical tests.

The object of future efforts will be a more extended validation of CATHARE-HLM to test the code capability in reproducing data coming from selected experimental campaigns and in comparison to the RELAP5 code version of ENEA. In particular, the CATHARE-HLM will be assessed on experimental data from the HELIOS Loop, released in the framework of the OECD/NEA LACANES Benchmark [5] by means of code-to-data comparison and code-to-code benchmark against RELAP5.

2. THE CATHARE CODE

CATHARE (Code for Analysis of THERmalhydraulics during an Accident of Reactor and safety Evaluation) is a T/H system code employed for safety analysis of water reactor, management of accidental scenario but also for the definition of operational procedures and to support the licensing of a NPP. The code is born in the 1979 and represent a collaboration among the CEA (Commissariat à l'Énergie Atomique), IRSN (Institut de Radioprotection et de Sûreté Nucléaire), EDF (Électricité de France) and AREVA NP.

The possible application may include the development of components and entire systems, in fact, thanks to its flexible modular structure, it can be used to in applications ranging from simple experimental test facility up to large and complex installation like nuclear power plant. Other application may be the definition and assessment of operative and emergency procedures, studies on new reactors and facilities as well as the support of the preparation of experimental campaigns. The “best-estimate” CATHARE code is used to simulate accidental scenario such as small, intermediate and large break LOCA, failure of steam generators and almost all the accidental sequences. Moreover, it is used in the nuclear power plant simulators and is capable to provide tools for uncertainties evaluation.

The CATHARE code treat the thermal-hydraulics of fluids mainly in one-dimensional motion flow with a two-phase model (liquid and gas) solving balance equations for mass, momentum and energy for each phase in the six main variables: liquid and gas enthalpy (H_L , H_G), liquid and gas velocity (V_L , V_G), pressure (P) and void fraction (α) with further optional equation to treat the transport of non-condensable gases (up to four) and radiochemical species (up to twelve). Moreover, the code is provided of closure relations to consider the conservation of mass, momentum and heat exchanged between the two phases and between each phase and the walls.

The space is discretized with a finite volume scheme in the balance equations of mass and energy and with a finite difference scheme for what regards the momentum equations. The time discretization use an implicit numerical scheme for 0D and 1D modules and a semi-implicit scheme in case of 3D elements including inter-phase exchange, pressure and convective terms. The system resolution is based on an iterative method of Raphson-Newton. Thanks to its robustness and reliability, the code allows to obtain a good compromise between precision and calculation time efficiency giving also many advantages in the extension to other application but LWR systems. As a matter of fact, the numerical solver is generic and the existing tools for pre- and post-processing can be used for all applications. Basic modeling features, like circuits with heat exchangers, various hydraulic elements, valves, walls, already exist, are well consolidated, and can be used for generic purpose. This is the reason why the new capabilities will be integrated as independent options in a unique standard version of the code respecting the same stringent procedures for quality assurance, in order to minimize development and maintenance costs.

3. APPROACH TO THE CATHARE MODIFICATIONS

The strategy followed for the development of CATHARE aims at minimize the users' effects building a reliable code, thanks to a great assessment efforts, with efficient maintenance process. To achieve these goals CATHARE has been developed as a single version multi-purpose multi-reactor code for all applications.

The code versions consist of:

- full versions (or major releases) where is introduced new functionalities or modifications on numerical aspects
- modified versions (or update) that correct the bugs found in the full versions.

Without going in deep in the CATHARE versioning, at the time when the implementation of lead and LBE are made, was:

- *CATHARE 2 V2.5_2mod2.1*, the reference full version
- *CATHARE 2 V2.5_2mod4.1*, the last update version released
- *CATHARE 2 V2.5_2mod5.1*, the forthcoming update release.

Pursuing the development philosophy of the code where each official release must be verified and validated, the new fluids have been implemented in a “service version” of CATHARE i.e. the *development version*, restricted to the developers. Nevertheless, the subroutine that will be added/modified could be used in any released version as mask files for CATHARE thermal-hydraulic computation, in other words, as FORTRAN files placed in the run directory that are able to substitute the original ones or add user features.

In the future, the code with its new fluids characteristic will be assessed against data that comes from experimental facilities such as:

- CIRCE – Facility located at the ENEA Brasimone laboratories to test the enhanced circulation by gas injection in LBE.
- MEGAPIE – PSI facility for test of LBE liquid metal spallation target of relevance for accelerator driven systems.
- HELIOS – Korean LBE integral test facility in natural and forced convection, object of international code benchmarking activity LACANES.

In particular, as a first step, the data coming from HELIOS loop will be used in forthcoming test activities, taking advantage of the ENEA participation on the benchmark with its own RELAP5 modified version.

In the present report will be discussed only simple analytical test cases.

After a period in which the modifications will be assessed, the subroutines should be ready to be included in the coming full version *CATHARE 2 V2.5_3mod2.1* whose release is scheduled in the year 2012.

Since the implementation of the sodium, CATHARE has been widely modified to become a multi-fluid code. This means that the efforts to add further fluids in the code have been greatly simplified and the way has been already traced. Most of the following work takes advantage of the work done with the sodium.

3.1. Thermodynamic properties in CATHARE

The thermodynamic properties that have been calculated for the thermodynamic subroutines of the different fluids are:

- Density $\rho(H,P)$
- Specific Heat $c_p(H,P)$
- Conductivity $\lambda(H,P)$
- Temperature $T(H,P)$
- Viscosity $\mu(H,P)$
- Enthalpy at saturation $H_{sat}(P)$
- Temperature at saturation $T_{sat}(P)$
- Surface tension $\sigma(H,P)$

whereas ρ , c_p , λ , T , μ and H_{sat} are properties characteristic of each phase (liquid and gas), T_{sat} and σ are independent of phases [6].

For each of these properties has been calculated the partial derivatives against pressure and enthalpy used in the building of the Jacobian matrix, follows that the functions (correlations) and their first degree derivatives must be continue in the domain of pressure and enthalpy.

Several conditions must be met:

- Elementary conditions: $\rho > 0$, $c_p > 0$, $\lambda > 0$, $T > 0$, $\mu > 0$, $T_{sat} > 0$, $\sigma > 0$
- Continuity of the functions and their derivatives in the domain
- Sign conditions on the derivatives: $\partial T / \partial H > 0$, $\partial \rho / \partial H < 0$, $\partial \rho / \partial P > 0$
- Continuity at saturation: $T_V(H_{V sat}(P), P) = T_L(H_{L sat}(P), P) = T_{sat}(P)$ and in particular:
 $T_{sat}(P_c) = T(P_c, H_c) = T_c$

To create the interpolation functions of the physical properties, a first analysis can consists in calculate a certain number of function $f(H)$ at constant pressure and $f(P)$ at constant enthalpy, to obtain the general curves shape in the domain space. Considering, as instance, the density:

$$\rho(H,P) = f(H,P) \quad \text{in the monophasic domain}$$

$$\rho(H,P) = f(H_{sat},P) + (H - H_{sat}) \cdot g(H_{sat},P) \quad \text{in the diphasic domain}$$

Where g function is a “terme de rappel”.

Starting from the analytical expression of the saturation temperature T_{sat} function of pressure, it can be defined the enthalpy intersecting the surface $H(T,P)$ and the saturation curve. This method assures the continuity on the vapour domain and the correctness of the function against those tables in literature.

Presence of non-condensable in the gas phase

The fluid properties are calculated:

- For the liquid phase, in function of the total pressure P and liquid temperature (T_L) and enthalpy (H_L)
- For the gas phase, in function of the partial pressure P_V , the gas temperature T_G and vapour enthalpy H_V (supposing that in presence of non-condensable the different gas have the same temperature but with its own enthalpy).

$P_V = P - (P_1 + \dots + P_4)$, where P_i is the partial pressure of the i -th non-condensable.

The P_i are defined as
 where:

$$P_i = \rho_i \cdot r_i \cdot T_G$$

$$\rho_i = X_i \cdot \rho_G$$

$$r_i = R / M_i$$

M_i molar mass of the element.

Through a double Newton method (subroutine FHSOLV) is calculated the P_V and H_V , therefore calculate the derivatives against P_V and H_V , and then in function of P , H_G and X_i . The non-condensables are considered gas perfect and their properties are mere function of temperature, supposed uniform:

$$T_G = T_V(P_V, H_V) = T_i(P_i, H_i)$$

The calculation of the fluid thermodynamic properties can be done in two different ways: with a call at polynomial function embedded in the CATHARE code or with a calling to an external module where the properties are calculated by interpolation of tabulated values.

In our case the first method has been considered.

The interface inside CATHARE between these different ways to calculate the properties are:

- Sub-program to call the functions
- Common files that contain the calculated variables and derivatives.

Never mind the fluid considered or the method adopted, the input variables to calculate thermodynamic and transport properties are the main variables: P (total pressure), H_L (enthalpy of liquid phase), H_G (enthalpy of gas phase), X_i (fraction of non-condensable). Same for the output variables: density, specific heat capacity, saturation temperature, viscosity, conductivity and surface tension.

The subroutines that compute the thermodynamic properties are called:

- In each iteration, before writing the system of equations to solve each module (volume, axial, etc.)
- By the walls, to evaluate the heat exchange condition between fluid and wall
- By the CATHARE gadgets (tee, sink, source, etc.)

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3.2. Sources to be modified

The subroutines to be modified [6] regard the following aspects:

- Fluid properties
- 1D Modules (axial elements) closure laws at scalar and vector points
- 0D Modules (volume elements) closure laws at scalar and vector points
- Thermal closure laws for the walls (in 1D and 0D modules)

The subroutines reside in the following position in the code tree:

../sources/hydc	<i>Folder that contains the characteristics of all the fluids.</i>
/eos	<i>Equation Of State folder</i>
/pb	<i>Lead thermodynamic properties</i>
/pb	<i>Lead thermodynamic properties</i>
/claws	<i>Closure Laws folder (Physical Laws)</i>
/pb	<i>Lead physical laws</i>
/pb	<i>Lead physical laws</i>

Fluid Properties

The main subroutines that drive the choice among the different fluids implemented in CATHARE are:

- **FHPFLD.f**, which is the pilot for the thermodynamic properties of the fluids:
This routine calls another routine **FHPfluid.f** which is the pilot for the thermodynamic properties (ρ_k , T_k , Cp_k , where k is liquid or gas) of each fluid.
- **FTRAFLD.f**, which is the pilot for the transport properties of all fluids:
This routine calls another routine **FTRAfluid.f** which is the pilot for the transport properties (λ_k , μ_k , σ where k is liquid or gas) of each fluid.

Note: To keep the following description as general as possible, the suffix fluid will be maintained; LBe got to be substituted in case of Lead-Bismuth Eutectic and Pb in case of lead.

Input parameters are pressure, enthalpy of liquid and gas, mass fractions of non-condensable gases. It is given below the calling tree for the calculation of thermodynamic and transport properties.

FHPfluid

Pilot of Thermodynamic Properties of the "fluid"(LBe/Pb).

FTSATPfluid

Properties calculation (T,H) at saturation in function of the pressure (TSP,HLSP,HVSP)

FTLIQfluid

TD properties calculation of the liquid phase (H_L, ρ_L, C_{pL}) in function of temperature and pressure, and relative derivative.

FHLIQfluid

TD properties calculation of the liquid phase (T_L, ρ_L, C_{pL}) in function of enthalpy and pressure, and relative derivative.

FTLIQfluid

...

FHVAPfluid

TD properties calculation of the gas phase (T_G, ρ_G, C_{pG}) with the hypothesis of gas perfect.

with non-condensable

FHINITfluid

Initialization of Pv and Hv for the Newton algorithm computation.

FTSATPfluid

Properties calculation (T,H) at saturation in function of the P_V (TSPV,HLSV,HVSV)

FHVAPfluid

...

FHSOLV

Calculation of Pv and Hv for system resolution (2 equations, 2 unknowns).

FTSATPfluid

Calculation of properties (T, H) after convergence.

FHVAPfluid

TD properties calculation of the gas phase (T_G, ρ_G, C_{pG}) in function of Pv and Hv after convergence, and relative derivatives.

FTRAfluid

Pilot of Thermodynamic Properties of the "fluid"(LBe/Pb).

FHLIQAfluid

Transport properties calculation of the liquid phase (λ_L, μ_L) in function of enthalpy and pressure, and relative derivative.

FHVAPAfluid

Transport properties calculation of the gas phase (λ_G, μ_G, σ) with the hypothesis of gas perfect.

The output structure of the property functions of sodium are maintained:

- **FSATH.H**: properties at saturation
- **FEAUH.H**: thermal properties (T_L, ρ_L, T_G, ρ_G). It is the same structure as the properties of water.
- **FTRANH.H**: Transport properties (λ_k, μ_k).

The CATHARE domain limits of the fluids functions are in the include **BOUNDS.H**. The output of the domain limits is addressed by routine **HINCIWR.f**.

The Newton iteration convergence criteria of fluids functions are in the include **CONVRG.H**. The include file **fluidPROP.H**, contains the physical domain, the constants and values, characteristic of each fluid required for the properties calculation and is invoked by **INIFLD.f** file that initialize the **BOUNDS.H** and **CONVRG.H**.

Moreover, a hydraulic module may need to occasionally calculated functions for one or more sub-modules. Therefore, the code CATHARE uses different callings for one-time calculation functions of the fluid:

- **FTSATPFLD.f** and **FPSATTFLD.f** : for the calculation of saturation properties, these subroutines call respectively **FTSATPfluid.f** (computation of $T_{sat}(P)$) et **FPSATTfluid.f** (computation of $P_{sat}(T)$).
- **FHVAPFLD.f** and **FHLIQFLD.f** : for the calculation of thermodynamic properties for gas and liquid phase, these subroutines call respectively **FHVAPfluid.f** et **FHLIQfluid.f**.
- **FTVAPFLD.f** and **FTLIQFLD.f** : for the calculation of the enthalpy function of the temperature needed by the Newton algorithm, these subroutines call respectively **FTVAPfluid.f** (computation of $H_v(T_G)$) and **FTLIQfluid.f** (computation of $H_L(T_L)$).

1D Module

It is given below the calling tree for the calculation of the closure laws at scalar points. The pilot file in this case is **ECOHYD.f**.

EDGSFLD

Pilot for computation of droplet diameter in scalar nodes.

EDGS

Computation for water, adopted as is for the new fluids

FDGSE

Computation of entrained droplet diameter

FDSBR

Computation of entrained droplet diameter (break up on the mixing grids)

EDGS(LBe/Pb)

To be used for other fluids when data will be available.

EQLEFLD

Pilot for computation of the liquid/interface heat transfer.

EQLE (Rev.5)

Computation for the water, adopted as is for the new fluids

EQLE(LBe/Pb)

To be used for other fluids when data will be available.

EQVEFLD

Pilot for computation of the vapour/interface heat transfer.

EQVENA (Rev.5)

Computation for the sodium, adopted as is for the new fluids

EQVE(LBe/Pb)

To be used for other fluids when data will be available.

FPHICRFLD

Pilot for computation of critical heat flux and the interface variables between fluid and walls.

FPHICRfluid

Computation for the new fluids (but same as sodium)

FPHICRNA

Computation for the sodium.

It is given below the calling tree for the calculation of the closure laws at vector points. The pilot file in this case is **ETJAC.f**.

EGRILVFLD	<i>Pilot for computation of the vector grids.</i>
EGRILVfluid	<i>Computation for the new fluids, but with calling to water or sodium subroutines</i>
EGRILV	<i>Computation for the water</i>

0D Module

It is given below the calling tree for the calculation of the closure laws at scalar points. The pilot file in this case is **VCOHYD.f**.

VQLEFLD	<i>Pilot for computation of the liquid/interface heat transfer.</i>
VQLE	<i>Computation for the water, adopted as is for the new fluids</i>
VQLE(LBe/Pb)	<i>To be used for other fluids when data will be available.</i>
VQVEFLD	<i>Pilot for computation of the vapour/interface heat transfer.</i>
VQVE	<i>Computation for the water, adopted as is for the new fluids</i>
VQVE(LBe/Pb)	<i>To be used for other fluids when data will be available.</i>
VMETRFLD	<i>Pilot for computation of the mass and energy transfer between subvolumes.</i>
VMETRfluid	<i>Computation for the new fluids, but with calling to water or sodium subroutines</i>
VMETR	<i>Computation for the water</i>
FPHICRFLD	<i>Pilot for computation of critical heat flux and the interface variables between fluid and walls.</i>
FPHICRfluid	<i>Computation for the new fluids (but same as sodium)</i>
FPHICRNA	<i>Computation for the sodium.</i>

It is given below the calling tree for the calculation of the closure laws at vector points. The pilot file in this case is **VGRILV.f**.

VGRILVFLD	<i>Pilot for computation of the vector grids.</i>
VGRILV	<i>Computation for the water, adopted as is for the new fluids</i>
VGRILV(LBe/Pb)	<i>To be used for other fluids when data will be available.</i>

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Walls

When walls are defined within a module, there is a class of subroutines common to all types of hydraulic components: WALLCOM.

Here it is given the calling tree for the wall/fluid heat flux calculation. The pilot file in this case is **WELFEC.f**.

FECPARFLD *for 1D module* *Pilot for computation of the fluid/wall heat transfer*
VECPARFLD *for 0D module*

FECPARfluid	<i>Computation of the wall heat flux to fluid for the new fluids in 1D and 0D module respectively</i>
VECPARfluid	
FPHIffluid	<i>Computation of heat flux from wall to liquid for the new fluid (same as sodium). Calculation of convective heat transfer coefficient liquid QPL (laminar - turbulent forced convection and natural convection) and nucleate boiling QPI (relationship from H₂O) Standard case is the correlation of Seban-Shimazaki, otherwise user may define a different correlation in COMPONEN(T) directive.</i>
FPHCOGfluid	<i>Computation of forced convection coefficient to gas (same as sodium).</i>
FPARZOfluid	<i>Computation of the zone index(same as water)</i>
FPHFIXfluid	<i>Computation of the heat transfer derivatives wall/liquid wall/gas in function of non-condensable mass fraction (same as water)</i>
FECPAR	<i>Computation for the water</i>

The **DICO** file, that is the list of directive and operator keywords, has to be adjourned with the new tags LEADBISM and LEAD used to invoke the new fluids LBE and lead respectively.

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3.3. Input keyword to run LBE and Lead

Temporarily, before the implementation of the lead and LBE in an official release, the instructions to be introduced in the input file to declare one of the new fluids as coolant are defined below.

The CALOPORT operator, used in data block only, defines the fluid to be considered by CATHARE. It must be specified during the construction of the circuit (see CIRCUIT operator). This fluid can be used along with non-condensable gases.

```

BEGIN DATA ;

CALOPORT = FLUID fluidname ;

           where fluidname =  LEAD           for
Lead
                               LEADBISM      for
LBE
.
.
.
Circuit1 = CIRCUIT elem1, elem2, elem3, .....,
CALOPORT ;

Circuit2 = CIRCUIT elema, elemb, elemc, ..... ;

ReactorName = REACTOR Circuit1 Circuit2 ;

END DATA ;

```

This instruction is unreferenced in the CATHARE's Dictionary.

4. HLM PROPERTIES

The correlations for the thermo-physical properties of the molten Lead-Bismuth Eutectic and lead at pressure of 0.1 MPa [4] with temperatures considered in Kelvin are:

Composition	Pb 44.5 – Bi 55.5	%wt.
Molar Mass	208.18	g mol ⁻¹
Melting Temperature	397.7	K
Latent Heat of Melting (Q melt)	3.86E+04	J kg ⁻¹
Boiling Temperature	1943	K
Latent Heat of Boiling (Q boil)	8.54E+05	J kg ⁻¹
Critical Temperature	4890	K
Critical Pressure	88.0E+06	Pa
Critical Density	2170	kg m ⁻³
Saturation Vapour Pressure	$p_{sat} = 1.11 \cdot 10^{10} \cdot \exp\left(-\frac{22552}{T}\right)$	Pa
Density	$\rho = 11096 - 1.3236 \cdot T$	kg m ⁻³
Specific Heat Capacity	$c_p = 159 - 2.72 \cdot 10^{-2} \cdot T + 7.12 \cdot 10^{-6} \cdot T^2$	J kg ⁻¹ K ⁻¹
Sound Velocity	$u_{sound} = 1773 + 0.1049 \cdot T - 2.873 \cdot 10^{-4} \cdot T^2$	m s ⁻¹
Elastic Modulus (Adiabatic)	$B_s = (35.18 - 1.541 \cdot 10^{-3} \cdot T - 9.191 \cdot 10^{-6} \cdot T^2) \cdot 10^9$	Pa
Thermal Conductivity	$\lambda = 3.61 + 1.517 \cdot 10^{-2} \cdot T - 1.741 \cdot 10^{-6} \cdot T^2$	W m ⁻¹ K ⁻¹
Dynamic Viscosity	$\eta = 4.94 \cdot 10^{-4} \cdot \exp\left(\frac{754.1}{T}\right)$	Pa s
Surface Tension	$\sigma = 0.437 - 6.6 \cdot 10^{-5} \cdot T$	N m ⁻¹
Thermal Expansion	$\beta_p = \frac{1}{(8383.2 - T)}$	K ⁻¹

Table 1 – LBE Thermo-Physical Properties from Handbook (2007).

Molar Mass	207.20	g mol ⁻¹
Melting Temperature	600.6	K
Latent Heat of Melting (Q melt)	2.38E+04	J kg ⁻¹
Boiling Temperature	2016	K
Latent Heat of Boiling (Q boil)	8.58E+05	J kg ⁻¹
Critical Temperature	4870	K
Critical Pressure	100.0E+06	Pa
Critical Density	2490	kg m ⁻³
Saturation Vapour Pressure	$p_{sat} = 6.5715 \cdot 10^9 \cdot \exp\left(-\frac{22247}{T}\right)$	Pa
Density	$\rho = 11367 - 1.1944 \cdot T$	kg m ⁻³
Specific Heat Capacity	$c_p = 175.1 - 4.961 \cdot 10^{-2} \cdot T + 1.985 \cdot 10^{-5} \cdot T^2 - 2.099 \cdot 10^{-9} \cdot T^3 - 1.524 \cdot 10^6 \cdot T^{-2}$	J kg ⁻¹ K ⁻¹
Sound Velocity	$u_{sound} = 1951.75 - 0.3423 \cdot T + 7.635 \cdot 10^{-5} \cdot T^2$	m s ⁻¹
Elastic Modulus (Adiabatic)	$B_s = (42.15 - 1.652 \cdot 10^{-2} \cdot T + 3.273 \cdot 10^{-6} \cdot T^2) \cdot 10^9$	Pa
Thermal Conductivity	$\lambda = 9.2 + 1.1 \cdot 10^{-2} \cdot T$	W m ⁻¹ K ⁻¹
Dynamic Viscosity	$\eta = 4.55 \cdot 10^{-4} \cdot \exp\left(\frac{1069}{T}\right)$	Pa s
Surface Tension	$\sigma = 0.519 - 1.13 \cdot 10^{-4} \cdot T$	N m ⁻¹
Thermal Expansion	$\beta_p = \frac{1}{(9516.9 - T)}$	K ⁻¹

Table 2 – Lead Thermo-Physical Properties from Handbook (2007).

5. FLUID PROPERTIES

The simulation of multi-phase fluid needed by the CATHARE code, require the evaluation of the physical properties for liquid and vapour phase in function of pressure and enthalpy. For what regards the liquid phase thermo-physical properties, it can be stated that the data provided by the open literature is sufficient to assess a feasible set of properties especially in the technical range of temperatures (400÷1500 K) even if, in some cases discrepancies exists among different sources and somewhere the “best fit” correlation is based on very poor experimental data. On the contrary, in the case of vapour phase there is a real lack of any information due to the fact that there are not available experimental data. So that, the characteristics of vapour phase are largely unknowns both for lead and LBE. This issue has been overcome considering the vapour behaves as gas perfect, approach that was already used to implement the sodium properties [7]. So that, the vapour phase properties has been evaluated with an adaptation of subroutines used for sodium treatment.

5.1. Density

The density correlation, and in general all the properties correlations for the liquid metals considered, are defined as a merely function of temperature. This is not far from the real behavior of the liquid metals, where the pressure dependence of any material property could be considered widely negligible. Nevertheless, the CATHARE code need the pressure dependence to solve the balance equation, so that a very small effect of compressibility must be taken into account and, due to its very low value and temperature dependency, it has been considered constant.

The compressibility factor is:
$$\chi = -\frac{1}{V} \left(\frac{\partial V}{\partial P} \right)_T = -\frac{1}{\rho} \left(\frac{\partial}{\partial P} \frac{1}{\rho} \right)_T = -\rho \left(-\frac{1}{\rho^2} \frac{\partial \rho}{\partial P} \right)_T$$

$$\chi = \frac{1}{\rho_L} \left(\frac{\partial \rho_L}{\partial P} \right)_{T_L} \quad \text{where } \rho_L = \rho_L(P_0, T)$$

$$\text{and } P_0 = 0.1 \text{ MPa}$$

solving to find the liquid density:
$$\rho_L(P, T) = \rho_L(P_0, T) \cdot \exp(\chi(P - P_0))$$

To optimize the following properties relationship and derivatives, seems better to express the term $\rho_L(P_0, T)$, that in case of lead and LBE is a polynomial of first order, as an inverse polynomial function. In fact, the relations that involve enthalpy and heat capacity are function of the specific volume $V = 1/\rho$. The treatment of temperature function at denominator would make unnecessarily complicate the derivatives, so that from a regression of the following:

$$\rho_L^*(P_0, T) = \frac{1}{\rho_L(P_0, T)}$$

with a polynomial form of second order, it is obtained:

$$\rho_L(P, T) = \frac{\exp(\chi(P - P_0))}{\rho_L^*(P_0, T)} \quad \text{where: } \rho_L^*(P_0, T) = \sum_{i=0}^2 r_i \cdot T^i$$

The derivatives versus pressure and temperature:

$$\left(\frac{\partial \rho_L}{\partial P}\right)_{T_L} = \chi \cdot \rho_L$$

$$\left(\frac{\partial \rho_L}{\partial T_L}\right)_P = -\frac{\exp(\chi(P-P_0)) \cdot \sum_{i=0}^2 i \cdot r_i \cdot T^{i-1}}{(\sum_{i=0}^2 r_i \cdot T^i)^2}$$

The pressure and enthalpy derivatives are obtained with the thermo-physical properties derivation in Appendix B:

$$\left(\frac{\partial \rho_L}{\partial P}\right)_{H_L} = \left(\frac{\partial \rho_L}{\partial P}\right)_{T_L} + \left(\frac{\partial \rho_L}{\partial T_L}\right)_P \cdot \left(\frac{\partial T_L}{\partial P}\right)_{H_L}$$

$$\left(\frac{\partial \rho_L}{\partial H_L}\right)_P = \left(\frac{\partial \rho_L}{\partial T_L}\right)_P \cdot \left(\frac{\partial T_L}{\partial H_L}\right)_P$$

where the derivative of temperature versus the pressure at constant enthalpy, has been derived in Appendix C as:

$$\left(\frac{\partial T_L}{\partial P}\right)_{H_L} = -\left(\frac{\partial T_L}{\partial H_L}\right)_P \cdot \left(\frac{\partial H_L}{\partial P}\right)_{T_L}$$

and by definition: $\left(\frac{\partial T_L}{\partial H_L}\right)_P \equiv \frac{1}{C_{pL}}$

LBE

The density correlation in the Handbook is: $\rho(P_0, T) = 11096 - 1.3236 \cdot T$

and the polynomial regression of second order with its coefficients is:

$$\rho_L^*(P_0, T) = \sum_{i=0}^2 r_i^{LBE} \cdot T^i = 9.03 \cdot 10^{-5} + 1.003 \cdot 10^{-8} \cdot T + 2.01 \cdot 10^{-12} \cdot T^2$$

The regression introduce an approximation error in the density evaluation that is:

$$\varepsilon = \frac{\rho_{Handbook} - \rho_{polynomial}}{\rho_{Handbook}} \leq 0.3\% \quad \text{for } T < 2200^\circ\text{C}$$

well below the range of uncertainties in the Handbook's density correlation.

Lead

The density correlation in the Handbook is: $\rho(P_0, T) = 11367 - 1.1944 \cdot T$

and the polynomial regression of second order with its coefficients is:

$$\rho_L^*(P_0, T) = \sum_{i=0}^2 r_i^{Pb} \cdot T^i = 8.83 \cdot 10^{-5} + 8.0 \cdot 10^{-9} \cdot T + 1.8 \cdot 10^{-12} \cdot T^2$$

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The regression introduce an approximation error in the density evaluation that is:

$$\varepsilon = \frac{\rho_{Handbook} - \rho_{polynomial}}{\rho_{Handbook}} \leq 0.2\% \quad \text{for } T < 2200^{\circ}\text{C}$$

well below the range of uncertainties in the Handbook's density correlation.

5.2. Compressibility Factor

The compressibility factor has been considered constant and evaluated started from the adiabatic elastic modulus correlation, knowing that:

$$B_S = -V \left(\frac{\partial P}{\partial V} \right)_S \equiv \frac{1}{\chi_S} = \rho \cdot u_{sound}^2$$

Follow that:
$$\chi_S = \frac{1}{\rho \cdot u_{sound}^2}$$

At the respective melting temperature (397.7K for LBE, 600.6K for lead), the compressibility factors are:

$$\chi_{LBE} = 3.022 \cdot 10^{-11} \text{ Pa}^{-1}$$

$$\chi_{Pb} = 3.0 \cdot 10^{-11} \text{ Pa}^{-1}$$

5.3. Enthalpy and Specific Heat Capacity

The same approach carried-out in the formulation of density considering the compressibility has been adopted to build an expression of enthalpy, function of temperature and pressure, starting from the heat capacity correlation provided by the Handbook.

Considering the Maxwell thermodynamic relations and imposing the relations derived in Appendix A:

$$\left(\frac{\partial H}{\partial P} \right)_T = V - T \left(\frac{\partial V}{\partial T} \right)_P$$

$$\left(\frac{\partial Cp}{\partial P} \right)_T = -T \left(\frac{\partial^2 V}{\partial T^2} \right)_P$$

the specific volume V can be expressed in:

$$V = \frac{1}{\rho} = \rho_L^*(P_0, T) \cdot e^{-\chi(P-P_0)} \quad \text{where: } \rho_L^*(P_0, T) = \sum_{i=0}^2 r_i \cdot T^i$$

If $P = P_0$, H_L could be expressed with the following:

$$H_L(P, T) = H_0 + \int_{T_0}^{T_L} Cp_0(T) \cdot dT + \int_{P_0}^P \left[V - T \left(\frac{\partial V}{\partial T} \right)_P \right] \cdot dP$$

where: $Cp_0(T) = \sum_{i=0}^2 c_i \cdot T^i$

LBE

The correlation for heat capacity of lead-bismuth eutectic is a polynomial of second order:

$$H_L = H_0 + \int_{T_0}^{T_L} \sum_{i=0}^2 c_i \cdot T^i \cdot dT + \int_{P_0}^P [\sum_{i=0}^2 r_i \cdot T^i \cdot e^{-\chi(P-P_0)} - T \cdot \sum_{i=0}^2 i \cdot r_i \cdot T^{i-1} \cdot e^{-\chi(P-P_0)}] \cdot dP$$

$$H_L = H_0 + \int_{T_0}^{T_L} \sum_{i=0}^2 c_i \cdot T^i \cdot dT + [\sum_{i=0}^2 r_i \cdot T^i - T \cdot \sum_{i=0}^2 i \cdot r_i \cdot T^{i-1}] \cdot \int_{P_0}^P e^{-\chi(P-P_0)} \cdot dP$$

$$H_L = H_0 + \sum_{i=0}^2 \frac{1}{i+1} \cdot c_i \cdot T^{i+1} + [\sum_{i=0}^2 r_i \cdot T^i - T \cdot \sum_{i=0}^2 i \cdot r_i \cdot T^{i-1}] \cdot \frac{e^{-\chi(P-P_0)} - 1}{-\chi}$$

where $H_0 = H_L(P_0) = Cp(T_{melt}) \cdot T_{melt} + \mathcal{L}_{melt} = 9.798 \cdot 10^4 \text{ J/kg}$

and \mathcal{L}_{melt} = latent heat at melting of LBE

By definition $Cp_L = \left(\frac{\partial H_L}{\partial T_L}\right)_P$, hence the derivatives of enthalpy versus pressure and temperature are:

$$\left(\frac{\partial H_L}{\partial P}\right)_{T_L} = [r_0 - r_2 \cdot T^2] \cdot e^{-\chi(P-P_0)}$$

$$\left(\frac{\partial H_L}{\partial T_L}\right)_P = Cp_L = \sum_{i=0}^2 c_i \cdot T^i + [2 \cdot r_2 \cdot T] \cdot \frac{e^{-\chi(P-P_0)} - 1}{\chi}$$

The derivatives of the specific heat capacity versus pressure and temperature are:

$$\left(\frac{\partial Cp_L}{\partial P}\right)_{T_L} = -2 \cdot r_2 \cdot T \cdot e^{-\chi(P-P_0)}$$

$$\left(\frac{\partial Cp_L}{\partial T_L}\right)_P = \sum_{i=0}^2 i \cdot c_i \cdot T^{i-1} + 2 \cdot r_2 \cdot \frac{e^{-\chi(P-P_0)} - 1}{\chi}$$

Lead

The formulation of correlation for heat capacity of lead is slightly different from that of LBE, namely of a kind:

$$Cp = \sum_{i=0}^3 d_i \cdot T^i + d_4 \cdot T^{-2}$$

reminding that in this case the coefficients r_i are those referred to lead:

$$H_L = H_0 + \sum_{i=0}^3 \frac{1}{i+1} \cdot d_i \cdot T^{i+1} - d_4 \cdot T^{-1} + [\sum_{i=0}^2 r_i \cdot T^i - T \cdot \sum_{i=0}^2 i \cdot r_i \cdot T^{i-1}] \cdot \frac{e^{-\chi(P-P_0)} - 1}{-\chi}$$

where: $H_0 = H_L(P_0) = Cp(T_{melt}) \cdot T_{melt} + \mathcal{L}_{melt} = 1.1256 \cdot 10^5 \text{ J/kg}$

and \mathcal{L}_{melt} = latent heat at melting of lead

By definition $Cp_L = \left(\frac{\partial H_L}{\partial T_L}\right)_P$, hence the derivatives of enthalpy are:

$$\left(\frac{\partial H_L}{\partial P}\right)_{T_L} = [r_0 - r_2 \cdot T^2] \cdot e^{-\chi(P-P_0)}$$

$$\left(\frac{\partial H_L}{\partial T_L}\right)_P = Cp_L = \sum_{i=0}^3 d_i \cdot T^i + d_4 \cdot T^{-2} + [2 \cdot r_2 \cdot T] \cdot \frac{e^{-\chi(P-P_0)} - 1}{\chi}$$

The derivatives of the specific heat capacity versus pressure and temperature are:

$$\left(\frac{\partial Cp_L}{\partial P}\right)_{T_L} = -2 \cdot r_2 \cdot T \cdot e^{-\chi(P-P_0)}$$

$$\left(\frac{\partial Cp_L}{\partial T_L}\right)_P = \sum_{i=0}^3 i \cdot d_i \cdot T^{i-1} - 2 \cdot d_4 \cdot T^{-3} + 2 \cdot r_2 \cdot \frac{e^{-\chi(P-P_0)} - 1}{\chi}$$

And then, for both liquid metals, the derivatives versus pressure and enthalpy are (Appendix B):

$$\left(\frac{\partial Cp_L}{\partial P}\right)_{H_L} = \left(\frac{\partial Cp_L}{\partial P}\right)_{T_L} + \left(\frac{\partial Cp_L}{\partial T_L}\right)_P \cdot \left(\frac{\partial T_L}{\partial P}\right)_{H_L}$$

$$\left(\frac{\partial Cp_L}{\partial H_L}\right)_P = \left(\frac{\partial Cp_L}{\partial T_L}\right)_P \cdot \left(\frac{\partial T_L}{\partial H_L}\right)_P$$

Where $\left(\frac{\partial T_L}{\partial P}\right)_{H_L} = -\left(\frac{\partial T_L}{\partial H_L}\right)_P \cdot \left(\frac{\partial H_L}{\partial P}\right)_{T_L}$ derived in Appendix C.

5.4. Thermal Conductivity

LBE

The thermal conductivity correlation for LBE is a second degree polynomial $\lambda_L = \lambda_L(T)$:

$$\lambda_L(T) = ZC0 + ZC1 \cdot T + ZC2 \cdot T^2 \text{ W m}^{-1} \text{ K}^{-1}$$

$$\left(\frac{\partial \lambda_L}{\partial P}\right)_{H_L} = \left(\frac{\partial \lambda_L}{\partial P}\right)_{T_L} + \left(\frac{\partial \lambda_L}{\partial T_L}\right)_P \cdot \left(\frac{\partial T_L}{\partial P}\right)_{H_L} = (ZC1 + 2 \cdot ZC2 \cdot T) \cdot \left(\frac{\partial T_L}{\partial P}\right)_{H_L}$$

$$\left(\frac{\partial \lambda_L}{\partial H_L}\right)_P = \left(\frac{\partial \lambda_L}{\partial T_L}\right)_P \cdot \left(\frac{\partial T_L}{\partial H_L}\right)_P = (ZC1 + 2 \cdot ZC2 \cdot T) \cdot \left(\frac{\partial T_L}{\partial H_L}\right)_P$$

Lead

The thermal conductivity correlation for LBE is a first degree polynomial where $\lambda_L = \lambda_L(T)$:

$$\left(\frac{\partial \lambda_L}{\partial P}\right)_{H_L} = \left(\frac{\partial \lambda_L}{\partial P}\right)_{T_L} + \left(\frac{\partial \lambda_L}{\partial T_L}\right)_P \cdot \left(\frac{\partial T_L}{\partial P}\right)_{H_L} = ZC1 \cdot \left(\frac{\partial T_L}{\partial P}\right)_{H_L}$$

$$\left(\frac{\partial \lambda_L}{\partial H_L}\right)_P = \left(\frac{\partial \lambda_L}{\partial T_L}\right)_P \cdot \left(\frac{\partial T_L}{\partial H_L}\right)_P = ZC1 \cdot \left(\frac{\partial T_L}{\partial H_L}\right)_P$$

5.5. Viscosity

LBE

The viscosity correlation for both liquid metals have an exponential form as:

$$\mu_L(T) = PMU1 \cdot \exp\left(\frac{PMU2}{T}\right) \quad [\text{Pa s}]$$

The derivatives versus pressure and enthalpy are:

$$\left(\frac{\partial \mu_L}{\partial P}\right)_{H_L} = \left(\frac{\partial \mu_L}{\partial P}\right)_{T_L} + \left(\frac{\partial \mu_L}{\partial T_L}\right)_P \cdot \left(\frac{\partial T_L}{\partial P}\right)_{H_L} = -\frac{PMU2}{T^2} \cdot \mu_L \cdot \left(\frac{\partial T_L}{\partial P}\right)_{H_L}$$

$$\left(\frac{\partial \mu_L}{\partial H_L}\right)_P = \left(\frac{\partial \mu_L}{\partial T_L}\right)_P \cdot \left(\frac{\partial T_L}{\partial H_L}\right)_P = -\frac{PMU2}{T^2} \cdot \mu_L \cdot \left(\frac{\partial T_L}{\partial H_L}\right)_P$$

5.6. Saturation Condition

For both liquid metals, the saturation curve has the form:

$$P_{sat}(T) = At \cdot \exp\left(\frac{Bt}{T}\right) \quad [\text{Pa}] \quad (\text{Bt is a negative coefficient})$$

its inversed form and derivative, used by the Raphson-Newton solution method, are:

$$T_{sat}(P) = \frac{Bt}{\ln\left(\frac{P}{At}\right)} \quad [\text{K}]$$

$$\frac{\partial T_{sat}}{\partial P} = \frac{Bt}{\ln\left(\frac{P}{At}\right)} \cdot \frac{1}{P \cdot \ln\left(\frac{P}{At}\right)}$$

5.7. Surface Tension

For both metals, the surface tension has the form:

$$\sigma(T) = SIO - SN \cdot T \quad [\text{N m}^{-1}]$$

$$\frac{\partial \sigma}{\partial P} = \frac{\partial \sigma}{\partial T_{sat}} \cdot \frac{\partial T_{sat}}{\partial P} = -SN \cdot \frac{Bt}{\ln\left(\frac{P}{At}\right)} \cdot \frac{1}{P \cdot \ln\left(\frac{P}{At}\right)}$$

The surface tension calculated at the saturation temperature of the vapour partial pressure has been maintained unchanged.

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Note: on the CATHARE derivative rules.

The derivatives could be tagged with a number from 1 to 6, meaning respectively that the property taken into account is derivate in function of one of the main variables:

1 → P	pressure
2 → H _L (or T _L)	enthalpy (temperature) of liquid
3 → H _V (or T _V)	enthalpy (temperature) of vapour
4 → α	void fraction
5 → v _L	velocity of liquid
6 → v _V	velocity of vapour

Where the derivations in function of temperature are made in FTLIQ..., FTVAP..., etc. subroutines, in function of enthalpy in FHLIQ..., FHVAP..., etc. subroutines.

6. SUBROUTINE MODIFICATION

- FTLIQfluid.f

The input variables are pressure and temperature supplying the density, enthalpy and heat capacity of liquid phase and their derivatives.

$$\left\{ \begin{array}{l} \rho_L(P, T) \equiv RL \\ \left(\frac{\partial \rho_L}{\partial P} \right)_{T_L} \equiv DRL1^{(T)} \\ \left(\frac{\partial \rho_L}{\partial T_L} \right)_P \equiv DRL2^{(T)} \end{array} \right.$$

$$\left\{ \begin{array}{l} H_L(P, T) \equiv HL \\ \left(\frac{\partial H_L}{\partial P} \right)_{T_L} \equiv DHL1^{(T)} \\ \left(\frac{\partial H_L}{\partial T_L} \right)_P \equiv DHL2^{(T)} \equiv Cp_L \end{array} \right.$$

$$\left\{ \begin{array}{l} Cp_L \equiv DHL2^{(T)} \\ \left(\frac{\partial Cp_L}{\partial P} \right)_{T_L} \equiv DCPL1^{(T)} \\ \left(\frac{\partial Cp_L}{\partial T_L} \right)_P \equiv DCPL2^{(T)} \end{array} \right.$$

- FHLIQfluid.f

The input variables are pressure and enthalpy supplying the temperature, density, heat capacity and thermal expansion coefficient of liquid phase and their derivatives. The superscript (T) means that the value comes from the calling of FTLIQfluid.f subroutine.

$$\left\{ \begin{array}{l} \left(\frac{\partial T_L}{\partial P} \right)_{H_L} \equiv DTL1 = - \left(\frac{\partial T_L}{\partial H_L} \right)_P \cdot \left(\frac{\partial H_L}{\partial P} \right)_{T_L} = - \frac{DHL1^{(T)}}{DHL2^{(T)}} \\ \left(\frac{\partial T_L}{\partial H_L} \right)_P \equiv DTL2 = \frac{1}{c_{pL}} = \frac{1}{DHL2^{(T)}} \end{array} \right.$$

$$\left\{ \begin{array}{l} \left(\frac{\partial c_{pL}}{\partial P} \right)_{H_L} \equiv DCPL1 = DCPL1^{(T)} + DCPL2^{(T)} \cdot DTL1 \\ \left(\frac{\partial c_{pL}}{\partial H_L} \right)_P \equiv DCPL2 = DCPL2^{(T)} \cdot DTL2 \end{array} \right.$$

$$\left\{ \begin{array}{l} \left(\frac{\partial \rho_L}{\partial P} \right)_{H_L} \equiv DRL1 = DRL1^{(T)} + DRL2^{(T)} \cdot DTL1 \\ \left(\frac{\partial \rho_L}{\partial H_L} \right)_P \equiv DRL2 = DRL2^{(T)} \cdot DTL2 \end{array} \right.$$

$$\left\{ \begin{array}{l} \left(\frac{\partial^2 \rho_L}{\partial H_L^2} \right)_P \equiv D2RLDHL2 = - \frac{1}{c_{pL}^2} \cdot \left(\frac{\partial \rho_L}{\partial T_L} \right)_P \cdot \left(\frac{\partial c_{pL}}{\partial H_L} \right)_P = -DTL2^2 \cdot DRL2^{(T)} \cdot DCPL2 \\ \left(\frac{\partial}{\partial P} \left(\frac{\partial \rho_L}{\partial H_L} \right)_P \right)_{H_L} \equiv D2RLDHLDP = \chi \cdot DTL2^2 \cdot DRL2^{(T)} \cdot DCPL1 \end{array} \right.$$

Thermal expansion is a simple function of density and has been kept as is, in fact:

$$\beta(T) = \frac{1}{V} \cdot \left(\frac{\partial V}{\partial T} \right)_P = - \frac{1}{\rho_L} \cdot \left(\frac{\partial \rho_L}{\partial T_L} \right)_P = - \frac{1}{\rho_L} \cdot \left(\frac{\partial \rho_L}{\partial H_L} \right)_P \cdot \left(\frac{\partial H_L}{\partial T_L} \right)_P$$

$$\left\{ \begin{array}{l} \beta_L(T) \equiv BETAL = - \frac{1}{RL} \cdot \frac{DRL2}{DTL2} \\ \left(\frac{\partial \beta_L}{\partial P} \right)_{H_L} \equiv DBETAL1 = BETAL \cdot \left(\frac{DCPL1}{CPL} - \frac{DRL1}{RL} + \frac{D2RLDHLDP}{DRL2} \right) \\ \left(\frac{\partial \beta_L}{\partial H_L} \right)_P \equiv DBETAL2 = BETAL \cdot \left(\frac{DCPL2}{CPL} - \frac{DRL2}{RL} + \frac{D2RLDHL2}{DRL2} \right) \end{array} \right.$$

- FHLIQAfluid.f

The input variables are pressure, enthalpy, temperature and its derivatives, density and its derivatives supplying the conductivity and dynamic viscosity of liquid phase and their derivatives.

$$\left\{ \begin{array}{l} \lambda_L(T) \equiv TLAL \\ \left(\frac{\partial \lambda_L}{\partial P}\right)_{H_L} \equiv DTLAL1 \\ \left(\frac{\partial \lambda_L}{\partial H_L}\right)_P \equiv DTLAL2 \end{array} \right.$$

$$\left\{ \begin{array}{l} \mu_L(T) \equiv TMUL \\ \left(\frac{\partial \mu_L}{\partial P}\right)_{H_L} \equiv DTMUL1 \\ \left(\frac{\partial \mu_L}{\partial H_L}\right)_P \equiv DTMUL2 \end{array} \right.$$

- FTSATPfluid.f

This routine characterizes the properties at saturation conditions and is common to both the variable systems: enthalpy-mass fractions and temperature-partial pressures. The input variables are pressure and mass fraction of non-condensable supplying the temperatures, enthalpy of liquid and vapour and their derivatives in function of partial pressure.

$$\left\{ \begin{array}{l} T_{sat}(P_V) \equiv TSPV \quad \text{without non-condensable } P_V = P \\ \left(\frac{\partial T_{sat}}{\partial P_V}\right)_H \equiv DTSPVV \\ \left(\frac{\partial H_{L,sat}}{\partial P_V}\right)_H \equiv DHLSVV = DHL1^{(T)} + DHL2^{(T)} \cdot DTSPVV \\ H_{V,sat}(P_V) = HVSV = HLSV + DELTAHV \quad \text{DELTAHV is the latent heat} \\ \left(\frac{\partial H_{V,sat}}{\partial P_V}\right)_H \equiv DHVSVV = DHLSVV \end{array} \right.$$

Since the change of the subroutine argument:

$$\begin{aligned} DHL1^{(T)} &= DHLSVV \\ DHL2^{(T)} &= DHLSVTV \end{aligned}$$

- *fluidPROP.H* (PBBIPROP.H and PBPROP.H)

This routine collects all the properties coefficients characteristic of the fluids, such as:

- molar mass
- critical point
- saturation characteristics
- physical domain of pressure, temperature and enthalpy
- properties of the liquid and vapour phase
- etc.

7. HEAT TRANSFER CORRELATION

Since the very beginning of the investigation upon HLM as coolant for the future NPP generation, in the frame of several European projects, the heat transfer correlations to be adopted for the treatment of HLM is the object of an extended evaluation campaign both with system codes and CDF codes to assess their results against experimental data [8]. The discussions over this issue are still going on. In particular, a lot of efforts have been done to find the best heat transfer correlation to simulate the heat exchange in rod bundles. Far to be a solved issue, in the frame of the implementation of HLM in CATHARE has been decided to keep open as much as possible this matter, hence the Seban-Shimazaki correlation has been adopted as the general correlation to be used in 1D and 0D module, modifying the original Spukinski correlation adopted for sodium respectively in the subroutines *FECPARfluid.f* and *VECPARfluid.f*. The choice of this correlation is due mainly to the fact that it is the correlation implemented in RELAP5, thus to simplify the future comparisons between the two codes but also because the RELAP5 modified code has been already assessed against experimental data coming from MEGAPIE [9], CHEOPE and CIRCE facility [10], etc. The specific correlation for heat transfer in rod bundle (but also others general correlations) could be introduced as “user correlation” thanks to the *COMPONEN(T) operator* of CATHARE (for detailed description see the Dictionary of Operators and Directives). The general formulation for the Nusselt Number inside CATHARE, needed to evaluate the heat transfer coefficient, is:

$$Nu = a \cdot (Re^b + c) \cdot Pr^d \cdot (1 + e \cdot Re^f)^{0.1}$$

Within the *COMPONEN* operator can be defined the coefficient for laminar flow Nu_0 , the hydraulic diameter for Reynolds Number computation and each of the coefficients above for turbulent flow.

Each of the heat transfer correlation taken into account can be expressed in the same formulation as above. In the following table has been collected the correlations of our interest:

Seban-Shimazaki	○	$Nu = 5.0 + 0.025 \cdot Pe^{0.8}$
Ushakov	D	$Nu = 7.55 \cdot x - 20 \cdot x^{-13} + 0.041 \cdot x^{-2} \cdot Pe^{(0.56+0.19 \cdot x)}$
Zhukov (w/o spacers)	□	$Nu = 7.55 \cdot x - 14 \cdot x^{-5} + 0.007 \cdot Pe^{(0.64+0.246 \cdot x)}$
Mikityuk	D □	$Nu = 0.047 \cdot (1 - e^{-3.8 \cdot (x-1)}) \cdot (Pe^{0.77} + 250)$
Spukinski (Na reference)	○	$Nu = 4.82 + 0.0185 \cdot Pe^{0.827}$

Table 3 – Heat Transfer Correlation considered

where x is the pitch over diameter ratio: $x = p/D$

the Pectlet Numer is: $Pe = Re \cdot Pr$

with Re Reynolds Number
Pr Prandtl Number

and Nusselt number is: $Nu = (h \cdot D_h)/k$

with h heat transfer coefficient
 D_h hydraulic diameter
k wall conductivity

The coefficient to be introduced in the BLOCK DATA within the COMPONENT operator are:

	$Nu0$	a	b	d
Seban-Shimazaki	5.0	0.025	0.8	0.8
Ushakov	$7.55 \cdot x - 20 \cdot x^{-13}$	$0.041 \cdot x^{-2}$	$0.56 + 0.19 \cdot x$	$0.56 + 0.19 \cdot x$
Zhukov (no spacers)	$7.55 \cdot x - 14 \cdot x^{-5}$	0.007	$0.64 + 0.246 \cdot x$	$0.64 + 0.246 \cdot x$
Mikityuk	$0.047 \cdot (1 - e^{-3.8 \cdot (x-1)}) \cdot 250$	$0.047 \cdot (1 - e^{-3.8 \cdot (x-1)})$	0.77	0.77

Table 4 – Coefficients for User Heat Transfer Correlation ($c, e, f = 0$)

8. TESTS

In the previous chapters have been explained the various steps that have brought at the implementation of physical properties of LBE and lead in CATHARE code.

This final section aims to give a preliminary verification, even though doesn't claim to be comprehensive, of the coherence between the modifications made upon the subroutines and the reference physical properties contained in the Handbook.

Further assessment will be the object of future more extended analyses by means of code-to-data comparison and code-to-code benchmark to test the code capability in reproducing data coming from selected experimental campaigns and in comparison to the RELAP5 code.

8.1. Physical properties

The first test is conducted with the help of *VALUEFLD* directive of CATHARE that, from the command block, allow to access directly to the thermodynamic and transport properties of the main fluid of a circuit. The user provides as input the gas/liquid state variables supplying the corresponding properties.

The input information are:

- Pressure [Pa]
- Mass fraction of X_i non-condensable
- Enthalpy of liquid or gas [J/kg], or temperature of liquid or gas [°C]

The properties which can be obtained:

- Enthalpy of liquid/gas (J/kg)
- Temperature of liquid/gas (°C)
- Density of liquid/gas (kg/m^3)
- Specific heat of liquid/gas (J/kg/°C)
- Conductivity of liquid/gas (W/m/K)
- Viscosity of liquid/gas (kg/m s)
- Saturation temperature at total/partial steam pressure (°C)
- Saturation enthalpy of liquid/gas at total/ partial steam pressure (J/kg)
- Surface tension (N/m)
- Partial pressure of steam (Pa)
- Partial enthalpy of steam (J/kg)
- Partial density of steam (kg/m^3)
- Enthalpy of the i -th non-condensable gas (J/kg)

The directive allows to verify that the properties computed by the new subroutine are correspondent with those of correlations implemented.

Some cases have been launched for a cross-check. At first, the non-condensable gases are not considered and the fluid is LBE. The pressure is 2 bars with a liquid temperature of 300°C. The properties calculated in the first column of the Table 5 are correct in comparison with the correlations taken into account. In the second column has been reported the characteristics computed starting from the liquid enthalpy calculated in the previous test. This test allow to verify the correctness of the subroutine *FHLIQ_* in the computation of $H(T)$ and $T(H)$. It can

be seen that except some approximations the results are coherent with those obtained in the previous test. To be noted that the residual gas phase has been initialized at the temperature of saturation, same behavior happens with the water. In the particular case of the HLMS this could not be a problem because of the very high saturation temperatures, which allow to affirm that never a systems cooled by LBE or lead will work at such a high temperatures.

	X1FRACT 1.E-5			
	PRESSURE 2.E5		PRESSURE 5.E5	PRESSURE 2.E5
	LIQTEMP 300.	LIQH 185099.05	LIQTEMP 300.	LIQTEMP 600.
LIQUID ENTHALPY	185099.053333	185099.050000	185125.945	228031.0946
LIQUID TEMPERATURE	300.000000	299.999977	300	600
LIQUID DENSITY	10340.332490	10340.332520	10340.42624	9941.366193
LIQUID HEAT CAPACITY	145.749016	145.749017	145.7483249	140.6781924
LIQUID CONDUCTIVITY	11.732765	11.732765	11.73276539	15.5283629
LIQUID VISCOSITY	1.8413E-03	1.8413E-03	1.84E-03	1.17E-03
GAS TEMPERATURE	1791.331333	1791.331333	1980.3388	1791.331333
GAS DENSITY	2.425522	2.425522	5.555213378	2.425521786
SATURATION TEMP	1791.269122	1791.269122	1980.281604	1791.269122
SURFACE TENSION	0.300849	0.300849	0.288374289	0.300848988

Table 5 – LBE thermodynamic and transport properties calculated by CATHARE

In the third column has been reported the results of a liquid temperature of 300°C at a pressure of 5 bars. Comparing with the first column, it can be stated that a change in pressure have a negligible impact on the physical properties (mainly function of temperature), underlining the good implementation of pressure (with the compressibility factor) in the relationships.

The last column report the results at a temperature of 600°C at a pressure of 2 bars, just to verify the compliance with those expected at different temperature.

The same procedure and the same conclusions have been done for the lead which results are reported in the Table 6.

	X1FRACT 1.E-5			
	PRESSURE 2.E5		PRESSURE 5.E5	PRESSURE 2.E5
	LIQTEMP 400.	LIQH 185099.05	LIQTEMP 400.	LIQTEMP 700.
LIQUID ENTHALPY	223371.88727	223371.88700	223398.1324	266669.674
LIQUID TEMPERATURE	400.00	399.999998	400	700
LIQUID DENSITY	10581.94875	10581.94875	10582.04399	10226.04213
LIQUID HEAT CAPACITY	146.6959209	146.695921	146.695194	142.076362
LIQUID CONDUCTIVITY	16.60465	16.60464998	16.60465	19.90465
LIQUID VISCOSITY	2.23E-03	2.23E-03	2.23E-03	1.36E-03
GAS TEMPERATURE	1875.479198	1875.479198	2084.384117	1875.479198
GAS DENSITY	2.319559518	2.319559518	5.285048974	2.319559518
SATURATION TEMP	1875.40624	1875.40624	2084.316454	1875.40624
SURFACE TENSION	0.276214363	0.276214363	0.252607757	0.276214363

Table 6 – Lead thermodynamic and transport properties calculated by CATHARE

8.2. Vertical heated tube

In the following test, a heated pipe has been simulated with the characteristics:

Tube

- length $L = 3.0$ m discretized by 30 meshes
- flow area $A=0.1$ m²
- diameter $D = 0.357$ m

Pins

- pin number 100
- diameter $d = 0.01$ m
- length $l = 3$ m
- volumetric power $P_{vol} = 10^8$ W/m³

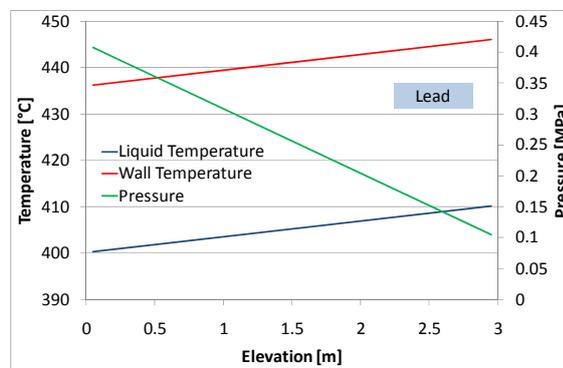
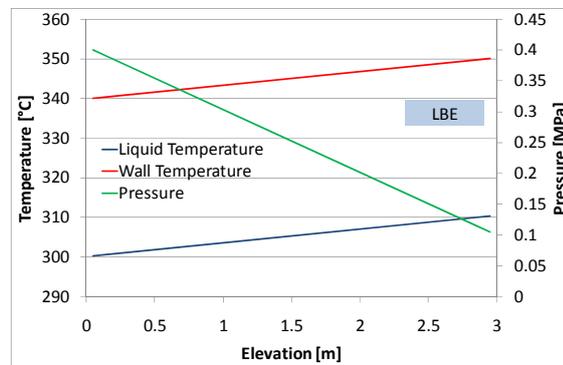
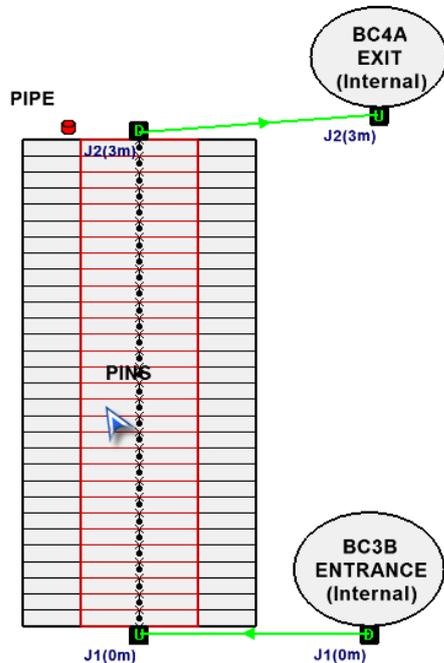
Boundary conditions

Entrance

- liquid/gas temperature $T_L = T_G = 300^\circ\text{C}$ (LBE) 400°C (Lead)
- void fraction $ALFA = 1.0E-5$
- liquid/gas velocity $V_L = V_G = 1.5$ m/s

Exit

- external pressure $P = 1.0E5$ Pa



Vertical heated pipe and temperature/pressure calculated

In the following will be discussed the case of LBE coolant, but the same treatment is valid even for lead. From CATHARE results for LBE, the heat-up through the core is 10.41°C with a mass flowrate 1551 kg/s. The wall temperature, evaluated with the default correlation

Seban-Shimazaki, results to be 40°C constantly higher than the fluid bulk temperature. The pressure variation follows the hydrostatic law from 4 bar up to 1 bar of the external pressure imposed with an average fluid density of 10333 kg/m³.

The analytical resolution of the pipe can be carried-out, knowing that:

$$P = \dot{m} c_p \Delta T$$

Where P is the power supplied by the pins, \dot{m} is the mass flowrate, c_p is the specific heat capacity and ΔT is the heat-up through the core.

The power supplied is:

$$P = P_{vol} \cdot V_{pin} \cdot 100 = 10^8 \cdot 2.356 \cdot 10^{-4} \cdot 100 = 2.356 \text{ MW}$$

The mass flowrate is known starting from the imposed liquid velocity:

$$\dot{m} = \rho \cdot v \cdot A = 10337 \cdot 1.5 \cdot 0.1 = 1550.55 \text{ kg/s}$$

where the density has been evaluated starting from the Handbook correlation at 300°C (573.15 K) and considering it approximatively constant. This assumption could be considered acceptable thanks to the small temperature variation expected along the pipe. A similar assumption has been made for the calculation of specific heat capacity that results, at 300°C, 145.75 J/kgK.

Now, it can be evaluated the heat-up of the LBE through the pipe, that is:

$$\Delta T = \frac{P}{\dot{m} c_p} = 10.43 \text{ }^\circ\text{C}$$

exactly what expected and calculated with CATHARE.

Also the temperature difference between the pin surface and coolant can be analytically estimated. Starting from the knowledge of the convective heat transfer coefficient:

$$Nu = \frac{h \cdot D_h}{\lambda} = 5.0 + 0.025 \cdot Pe^{0.8} \quad (\text{the Seban-Shimazaki correlation considered})$$

$$Pe = Re \cdot Pr = \frac{\rho \cdot v \cdot D_h}{\mu} \cdot \frac{\mu \cdot c_p}{\lambda} = \frac{\rho \cdot v \cdot D_h \cdot c_p}{\lambda} = 18024$$

where:

$$\begin{aligned} \rho_{(300^\circ\text{C})} &= 10337 \text{ kg/m}^3 \\ v &= 1.5 \text{ m/s} \\ D_h &= \frac{4A}{P} = \frac{4 \cdot 0.1}{3.14 + 1.12} = 0.0939 \text{ m (hydraulic diameter)} \\ c_{p(300^\circ\text{C})} &= 145.75 \text{ J/kgK} \\ \lambda_{(300^\circ\text{C})} &= 11.733 \text{ W/mK} \end{aligned}$$

Follows that: $Nu = 68.48 \Rightarrow h = \frac{Nu \cdot \lambda}{D_s} = 6306.7 \text{ W/m}^2\text{K}$

where D_s is the heating diameter: $D_s = \frac{4A}{P_s} = \frac{4 \cdot 0.1}{3.14} = 0.1274 \text{ m}$

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Now it is possible to calculate the temperature gap between the wall and the bulk:

$$P = h A \Delta T \quad \Rightarrow \quad \Delta T = \frac{2.356 \cdot 10^6}{9.42 \cdot 6306.7} \cong 40^\circ\text{C}$$

where P is the integral power generated by the A total surface area of the pins. The ΔT calculated is coherent with the CATHARE computation.

Also the results obtained with the numerical simulation for the lead case: the heat-up through the core 10.10°C , mass flowrate 1587 kg/s and the wall temperature 36°C constantly higher than the fluid bulk temperature, are in line in comparison to what is analytically expected.

CONCLUSIONS

In the frame of the ENEA/CEA STC agreement, the capability of the French system code CATHARE has been extended to simulate HLM reactors cooled by LBE and lead. The advantage to work on this code is that it has been already modified, in the recent past, to be multi-fluid and as a part of an European simulation platform (NURISP project) it is capable to provide an adequate support for future improvement and development.

Following as guideline the implementation procedure of sodium and thanks to the material properties collected in an Handbook issued by OECD-NEA, the thermodynamic and transport properties of LBE and lead has been introduced on the basis of experimental correlations with the possibility of future updates when new experimental evidences will be available.

The subroutines modified, that works as masks of CATHARE kernel, have been verified against very simple test with very good results. Some cross-checking runs with the help of *VALUEFLD* directive have shown a coherent evaluation of the thermodynamic and transport properties in comparison the experimental correlations introduced. The test carried-out with a vertical pipe heated by a rod bundle have been analytically solved shown a completely agreement against the results obtained with CATHARE, both regards the coolant heat-up through the pipe and regards the temperature difference between the rod-wall and bulk flow.

In particular, the latter has been calculated with the Seban-Shimazaki correlation, introduced as default heat transfer correlation for CATHARE, even if it is not the best correlation to evaluate convection heat exchange within rod bundles for LBE and lead fluids.

The object of future efforts will be a more extended validation of CATHARE-HLM to test the code capability in reproducing data coming from selected experimental campaigns and in comparison to the RELAP5 code version of ENEA. In particular, the CATHARE-HLM will be assessed on experimental data from the HELIOS Loop, released in the framework of the OECD/NEA LACANES Benchmark by means of code-to-data comparison and code-to-code benchmark against RELAP5.

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Appendix A

To calculate the derivative of the enthalpy in function of the pressure at constant temperature, it is known that:

$$\boxed{Cp = \left(\frac{\partial H}{\partial T}\right)_P}, \quad dH = TdS + VdP \quad \text{and} \quad dS = \left(\frac{\partial S}{\partial T}\right)_P dT + \left(\frac{\partial S}{\partial P}\right)_T dP.$$

Follow that $dH = T \left[\left(\frac{\partial S}{\partial T}\right)_P dT + \left(\frac{\partial S}{\partial P}\right)_T dP \right] + VdP = T \left(\frac{\partial S}{\partial T}\right)_P dT + \left[T \left(\frac{\partial S}{\partial P}\right)_T + V \right] dP$

but also $dH = \left(\frac{\partial H}{\partial T}\right)_P dT + \left(\frac{\partial H}{\partial P}\right)_T dP = Cp \cdot dT + \left(\frac{\partial H}{\partial P}\right)_T dP$

term by term $Cp = T \left(\frac{\partial S}{\partial T}\right)_P$ and $\left(\frac{\partial H}{\partial P}\right)_T = T \left(\frac{\partial S}{\partial P}\right)_T + V$

Moreover, from the Maxwell's relations $\left(\frac{\partial S}{\partial P}\right)_T = - \left(\frac{\partial V}{\partial T}\right)_P$

It is obtained $\boxed{\left(\frac{\partial H}{\partial P}\right)_T = V - T \left(\frac{\partial V}{\partial T}\right)_P}$

and the enthalpy could be rewritten as $dH = Cp \cdot dT + \left[V - T \left(\frac{\partial V}{\partial T}\right)_P \right] dP.$

To calculate the derivative of the heat capacity in function of the pressure at constant temperature:

$$dS = \left(\frac{\partial S}{\partial T}\right)_P dT + \left(\frac{\partial S}{\partial P}\right)_T dP = \frac{Cp}{T} dT - \left(\frac{\partial V}{\partial T}\right)_P dP$$

so that $\frac{Cp}{T} dT = dS + \left(\frac{\partial V}{\partial T}\right)_P dP$

deriving against pressure $\left(\frac{\partial(Cp/T)}{\partial P}\right)_T = - \left(\frac{\partial^2 V}{\partial T^2}\right)_P$

and finally $\boxed{\left(\frac{\partial Cp}{\partial P}\right)_T = -T \left(\frac{\partial^2 V}{\partial T^2}\right)_P}.$

Appendix B

Aiming to express the derivatives of thermophysical properties in function of pressure and enthalpy, the derivative of properties such as density (ρ), specific heat capacity (c_p), conductivity (λ) and viscosity (μ) both in liquid and vapour phase, could be expressed as follows, where X is the generic property.

$$dX = \left(\frac{\partial X}{\partial P}\right)_T dP + \left(\frac{\partial X}{\partial T}\right)_P dT$$

$$dX = \left(\frac{\partial X}{\partial P}\right)_T dP + \left(\frac{\partial X}{\partial T}\right)_P \cdot \left[\left(\frac{\partial T}{\partial P}\right)_H dP + \left(\frac{\partial T}{\partial H}\right)_P dH \right]$$

$$dX = \left[\left(\frac{\partial X}{\partial P}\right)_T + \left(\frac{\partial X}{\partial T}\right)_P \cdot \left(\frac{\partial T}{\partial P}\right)_H \right] dP + \left[\left(\frac{\partial X}{\partial T}\right)_P \cdot \left(\frac{\partial T}{\partial H}\right)_P \right] dH$$

At fixed enthalpy $\boxed{\left(\frac{\partial X}{\partial P}\right)_H = \left(\frac{\partial X}{\partial P}\right)_T + \left(\frac{\partial X}{\partial T}\right)_P \cdot \left(\frac{\partial T}{\partial P}\right)_H}$

At fixed pressure $\boxed{\left(\frac{\partial X}{\partial H}\right)_P = \left(\frac{\partial X}{\partial T}\right)_P \cdot \left(\frac{\partial T}{\partial H}\right)_P}$.

Appendix C

To calculate the derivative of the temperature in function of the pressure at constant enthalpy, it is known that:

$$dT = \left(\frac{\partial T}{\partial H}\right)_P dH + \left(\frac{\partial T}{\partial P}\right)_H dP \quad \text{and} \quad dH = \left(\frac{\partial H}{\partial T}\right)_P dT + \left(\frac{\partial H}{\partial P}\right)_P dP$$

replacing the dH expression in the first equation, follow that

$$dT = \left(\frac{\partial T}{\partial H}\right)_P \left(\frac{\partial H}{\partial T}\right)_P dT + \left[\left(\frac{\partial T}{\partial H}\right)_P \left(\frac{\partial H}{\partial P}\right)_T + \left(\frac{\partial T}{\partial P}\right)_H \right] dP \quad \text{and}$$

$$\left[\left(\frac{\partial T}{\partial H}\right)_P \left(\frac{\partial H}{\partial T}\right)_P - 1 \right] dT + \left[\left(\frac{\partial T}{\partial H}\right)_P \left(\frac{\partial H}{\partial P}\right)_T + \left(\frac{\partial T}{\partial P}\right)_H \right] dP = 0 .$$

Simplifying $\left(\frac{\partial T}{\partial H}\right)_P \left(\frac{\partial H}{\partial P}\right)_T + \left(\frac{\partial T}{\partial P}\right)_H = 0$

Hence $\boxed{\left(\frac{\partial T}{\partial P}\right)_H = - \left(\frac{\partial T}{\partial H}\right)_P \left(\frac{\partial H}{\partial P}\right)_T}$.