Phenomenology of Liquid Metal Thermal-Hydraulics

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1st October 1999

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1 Introduction

The cooling system of the Energy Amplifier (EA) is based on a Lead flow driven by natural circulation [1]. In the Energy Amplifier Demonstration Facility (EADF) a Lead-Bismuth eutectic is used and natural circulation, although enhanced through a gas injection system, is the pumping force for the cooling of both the target (only in the case of the window-type target) and the primary circuit[2].

Numerical simulation is extensively used for the design and analysis of these flows, using both commercial and in-house codes. However, liquid metals properties are very different from that of common fluids, so the physical models to be used in the simulations should be carefully assessed.

In general the numerical simulation of any kind of flow requires:

(i) the thermodynamic modelling of the fluid;

(ii) the fluid dynamics governing equations;

(iii) the turbulence modelling.

In this work the thermodynamic model for heavy liquid metals is presented, starting with the derivation of the equations of state for a general fluid from the basic laws of thermodynamics.

This thermodynamic model is then used for the analysis of a one-dimensional natural convection loop, in order to put in evidence the main physical mechanisms governing this particular kind of flow and the simplifications that can be applied to the one dimensional governing equations.

An extensive analysis of the tree-dimensional fluid dynamic governing equations and of the turbulence models for liquid metal flows can be found in [7] and [8] respectively.

2 Thermodynamics of Fluids

2.1 Overviews

The equilibrium state of a thermodynamic system can be described by one couple of state variables (one intensive and one extensive) for each way the system can exchange energy with the surrounding [3]. These variables are not all independent; in fact the number of degrees of freedom of the system is equal to the number N_e of energy exchange ways, the state variables being related by N_e *equations of state*.

For the purpose of the present study it is sufficient to consider the thermodynamic system as a fluid which can exchange pressure work and heat with the surrounding ($N_e = 2$; this is usually referred as $p\,v\,T$ system). The variables describing the work exchange are the *pressure* p ($[Pa]$, intensive) and the *volume* V ($[m^3]$, extensive); the heat exchange is described by the *temperature* T ($[K]$, intensive) and the *entropy* S ($[J/K]$, extensive). The extensive variables can be made independent of the mass of the system by using specific quantities like the *specific volume* v ($[m^3/Kg]$), or the *density* $\rho = 1/v$, and the *specific entropy* s ($[J/(Kg\,K)]$).

The four variables p, v, T and s are related by two equations of state of the type

$$\mathcal{F}(p, T, v) = 0\,, \tag{1}$$

$$\mathcal{G}(s, T, v) = 0 \quad \text{or} \quad \mathcal{G}(s, T, p) = 0 \tag{2}$$

which fully describe the thermodynamic behaviour of the system.

The *specific internal energy* e of the system is related to the other state variables by the first and second laws of thermodynamics. For an infinitesimal reversible transformation of a closed system they can be written as

$$de = \delta Q_{rev} - \delta W_{rev} = \delta Q_{rev} - p\,dv \qquad (3)$$

$$ds = \frac{\delta Q_{rev}}{T} \qquad (4)$$

where δQ_{rev} is the amount of heat received by the system undergoing a "quasi-static" reversible process. The symbol d refers to "perfect differentials" (i.e their integrals depend only on the initial and final states); the symbol δ refers to "imperfect differentials" (i.e their integrals depend on the thermodynamic precess type). Combination of Eqs. (3) and (4) yields

$$\boxed{de = T\,ds - p\,dv} \qquad (5)$$

Although this equation has been obtained with the assumption of reversible process in a closed system, it has general validity because only state variables appear in Eq. (5).

The *specific enthalpy* h is defined as

$$h = e + p\,v\,. \qquad (6)$$

Differencing Eq. (6) and considering Eq. (5) we obtain

$$\boxed{dh = T\,ds + v\,dp} \qquad (7)$$

Equations relating e or h to other two thermodynamic variables are obviously equivalent to Eqs. (1) and (2), and can be used as equations of state.

2.2 Equations of state

The equations of state for a $p\,v\,T$ thermodynamic system are deduced from experimental observation of the measurable quantities p, v and T. Sometimes the analytical form of Eqs. (1)-(2) can be found directly (in the case of gases); otherwise they can be deduced on the basis of experimental measurements of the following thermodynamic quantities:

i) The *thermal-expansion coefficient* β defined as

$$\beta = \frac{1}{v}\left(\frac{\partial v}{\partial T}\right)_p = -\frac{1}{\rho}\left(\frac{\partial \rho}{\partial T}\right)_p . \qquad (8)$$

ii) The *isothermal coefficient of compressibility* χ defined as

$$\chi = -\frac{1}{v}\left(\frac{\partial v}{\partial p}\right)_T = \frac{1}{\rho}\left(\frac{\partial \rho}{\partial p}\right)_T . \qquad (9)$$

iii) The *specific heat at constant volume* C_v or the *specific heat at constant pressure* C_p defined respectively as

$$C_v = \left(\frac{\delta Q}{dT}\right)_{dv=0} , \qquad (10)$$

$$C_p = \left(\frac{\delta Q}{dT}\right)_{dp=0} . \qquad (11)$$

The specific heats are related by the equation (see App. A.4)

$$\boxed{C_p - C_v = \frac{\beta^2\, T\, v}{\chi}} \tag{12}$$

In the case of liquids, a direct measurement of χ is very difficult; therefore, its value is deduced by measuring the speed of sound c and by using the relation [4]

$$c^2 = \frac{C_p}{C_v\, \chi\, \rho}\,. \tag{13}$$

The first equation of state (Eq. (1)) can be obtained by integrating the differential form of v as a function of T and p:

$$dv = \left(\frac{\partial\, v}{\partial\, T}\right)_p dT + \left(\frac{\partial\, v}{\partial\, p}\right)_T dp$$

which, taking in account definitions (8)-(9), can be written as

$$\frac{dv}{v} = \beta\, dT - \chi\, dp\,. \tag{14}$$

or, in terms of density

$$\frac{d\rho}{\rho} = -\beta\, dT + \chi\, dp\,. \tag{15}$$

The second equation of state (2) comes from the differential form of s, that is expressed in terms of C_v or C_p respectively as (see App. A.3)

$$ds \;=\; \frac{C_v}{T}\, dT + \frac{\beta}{\chi}\, dv\,, \tag{16}$$

$$ds \;=\; \frac{C_p}{T}\, dT - \beta\, v\, dp\,. \tag{17}$$

Therefore, the fluid is described in terms of the variables (T, v) by the system

$$\begin{bmatrix} dp \\ ds \end{bmatrix} = \begin{bmatrix} \beta/\chi & -1/(\chi\, v) \\ C_v/T & \beta/\chi \end{bmatrix} \begin{bmatrix} dT \\ dv \end{bmatrix} \tag{18}$$

and in terms of (T, p) by the system

$$\begin{bmatrix} dv \\ ds \end{bmatrix} = \begin{bmatrix} \beta\, v & -\chi\, v \\ C_p/T & -\beta v \end{bmatrix} \begin{bmatrix} dT \\ dp \end{bmatrix}\,. \tag{19}$$

The differential forms on the left-hand side of Eq. (18) and (19) are perfect differentials and consequently must satisfy the conditions $\partial^2/\partial T\partial v = \partial^2/\partial v\partial T$ and $\partial^2/\partial T\partial p = \partial^2/\partial p\partial T$ respectively. Hence, from Eq. (18) one obtains

$$\left(\frac{\partial\, \beta/\chi}{\partial\, v}\right)_T = -\frac{1}{v}\left(\frac{\partial\, 1/\chi}{\partial\, T}\right)_v\,, \tag{20}$$

$$\frac{1}{T}\left(\frac{\partial\, C_v}{\partial\, v}\right)_T = \left(\frac{\partial\, \beta/\chi}{\partial\, T}\right)_v \tag{21}$$

and from Eq. (19)

$$\left(\frac{\partial \beta v}{\partial p}\right)_T = -\left(\frac{\partial \chi v}{\partial T}\right)_p , \tag{22}$$

$$\frac{1}{T}\left(\frac{\partial C_p}{\partial p}\right)_T = -\left(\frac{\partial \beta v}{\partial T}\right)_p . \tag{23}$$

When making assumptions about the thermodynamic characteristics of a fluid one have to check if his model is congruent with the above conditions. If an expression for β, χ and C_v (or C_p) is known, Eqs. (18) (or (19)) can be integrated yielding the equations of state (1) and (2).

2.3 Equations for internal energy and enthalpy

Expressions relating the internal energy and the enthalpy to the couples of state variables (T, v) and (T, p) can be deduced as follows.

The relation $e = e(T, v)$ can be obtained from Eqs. (5) and (16), yielding

$$\boxed{de(T, v) = \left(\frac{\partial e}{\partial T}\right)_v dT + \left(\frac{\partial e}{\partial v}\right)_T dv = C_v\, dT + \left(\frac{\beta T}{\chi} - p\right) dv} \tag{24}$$

which can be integrated if an expression $p = p(T,\ v)$ is available from Eqs. (18). The expression $e = e(T, p)$ is given by (see App. A.5)

$$\boxed{de(T, p) = \left(\frac{\partial e}{\partial T}\right)_p dT + \left(\frac{\partial e}{\partial p}\right)_T dp = (C_p - \beta\, p\, v)\ dT - (\beta\, T - \chi\, p)\ v\, dp} \tag{25}$$

which can be integrated if an expression $v = v(T,\ p)$ is available from Eqs. (19).

The relation $h = h(T, p)$ can be obtained from Eqs. (7) and (17)

$$\boxed{dh(T, p) = \left(\frac{\partial h}{\partial T}\right)_p dT + \left(\frac{\partial h}{\partial p}\right)_T dp = C_p\, dT + (1 - \beta\, T)\, v\, dp} \tag{26}$$

which can be integrated if an expression $v = v(T,\ p)$ is available from Eqs. (19). The expression $h = h(T, v)$ is given by (see App. A.5)

$$\boxed{dh(T, v) = \left(\frac{\partial h}{\partial T}\right)_v dT + \left(\frac{\partial h}{\partial v}\right)_T dv = \left(C_v + \frac{\beta}{\chi} v\right) dT + \frac{1}{\chi}(\beta\, T - 1)\ dv}. \tag{27}$$

2.4 Integration of the differential state equations

The general differential equation of state for the thermodynamic variable F can be written as

$$dF = f(x, y)\, dx + g(x, y)\, dy \tag{28}$$

where x and y are two state variables and f and g are two functions of x and y. Being F a perfect differential the result of the integration does not depend on the integration path. Therefore the integration from (x_0, y_0) to (x, y) can be split in two integrations from (x_0, y_0) to (x, y_0) (with $y \equiv$ const) and from (x, y_0) to (x, y) (with $x \equiv$ const), yielding

$$\int_{(x_0,y_0)}^{(x,y)} dF = F(x, y) - F_0 = \int_{x_0}^{x} f(\tilde{x}, y_0)\, d\tilde{x} + \int_{y_0}^{y} g(x, \tilde{y})\, d\tilde{y} \tag{29}$$

where $F_0 = F(x_0, y_0)$ and the subscript 0 indicates a reference condition.

Usually, depending on the available expressions for β, χ, C_p and C_v (coming from experimental measurements), the integration is simpler for one state function rather then another. For example, if expressions for $C_v(T)$, $\beta(T, v)$ and $\chi(T, v)$ are available, it could be simpler integrating Eq. (24) rather than Eq. (25). An expression for $e(T, p)$ could then be found from the first equation of state in terms of $v(T, p)$.

2.5 Perfect Gas

As an example the perfect gas equations of state will be deduced with the above procedure. For a perfect gas $\beta = 1/T$, $\chi = v/(RT)$ and $C_v = C_v(T)$. From the first of Eqs. (18) we have

$$\left(\frac{\partial p}{\partial T}\right)_v = \frac{\beta}{\chi} = \frac{R}{v}$$
$$\left(\frac{\partial p}{\partial v}\right)_T = -\frac{1}{\chi\, v} = -\frac{RT}{v^2}\,.$$

Hence

$$p = p_0 + \int_{T_0}^{T} \frac{R}{v_0}\, dT - \int_{v_0}^{v} \frac{RT}{v^2}\, dv = p_0 - \frac{RT_0}{v_0} + \frac{RT}{v}$$

and finally, considering that $p_0 = \dfrac{RT_0}{v_0}$,

$$p = \frac{RT}{v} \tag{30}$$

which is the perfect gas equation of state.

Substituting the values of β,χ and C_v into Eq. (24) we obtain

$$de = C_v(T)\, dT + \left(\frac{RT}{v} - p\right) dv = C_v(T)\, dT \tag{31}$$

which implies

$$e = e(T) \tag{32}$$

that is the second equation of state for the perfect gas. The second equation of state in term of the entropy $s = s(T, v)$ (see Eq. (2)) can be derived integrating Eq. (5); in the case of the ideal gas ($C_v \equiv$ const) it is easy to verify that

$$s = s_0 + C_v \ln \frac{T}{T_0} + R \ln \frac{v}{v_0} \tag{33}$$

2.6 Fluids with constant β, χ and C_v

The assumption $\beta \equiv$ const and $\chi \equiv$ const are congruent with Eq. (20). Moreover, from Eq. (21), it follows $C_v = C_v(T)$. The integration of Eq. (14) yields

$$v\,(T, p) = v_0 \, \exp\left[\beta\,(T - T_0) - \chi\,(p - p_0)\right] \tag{34}$$

that is the first equation of state. If the further assumption

$$C_v \equiv \text{const}$$

is considered, the integration of Eq. (16) yields

$$s\,(T, v) = s_0 + C_v \, \ln \frac{T}{T_0} + \frac{\beta}{\chi}\,(v - v_0)\,. \tag{35}$$

which is the second equation of state. An expression for the internal energy as a function of T and v can be deduced from Eq. (24). One has

$$\left(\frac{\partial\, e}{\partial\, T}\right)_v = C_v \tag{36}$$

$$\left(\frac{\partial\, e}{\partial\, v}\right)_T = \left(\frac{\beta\, T}{\chi} - p\right) \tag{37}$$

The pressure p can be explicited from Eq. (34):

$$p(T, v) = p_0 + \frac{\beta}{\chi}\Delta T - \frac{1}{\chi}\ln\left(\frac{v}{v_0}\right) \tag{38}$$

where $\Delta T = T - T_0$. Substituting Eq. (38) into Eq. (37), one obtains

$$\left(\frac{\partial\, e}{\partial\, v}\right)_T = -p_0 + \frac{\beta}{\chi}\, T_0 + \frac{1}{\chi}\ln\left(\frac{v}{v_0}\right) \tag{39}$$

Substituting Eqs. (36) and (39) into Eq. (24) and integrating we obtain[1]

$$e(T, v) = e_0 + \int_{T_0}^{T} C_v \, dT + \int_{v_0}^{v} \left[\left(\frac{\beta}{\chi}\, T_0 - p_0\right) + \frac{1}{\chi}\ln\left(\frac{v}{v_0}\right)\right] \, dv \tag{40}$$

and, finally

$$\boxed{e\,(T, v) = e_0 + C_v\,\Delta T + \left(\frac{\beta\, T_0}{\chi} - p_0\right)\Delta v + \frac{v_0}{\chi}\left[\frac{v}{v_0}\,\ln\left(\frac{v}{v_0}\right) - \frac{\Delta v}{v_0}\right]\;.} \tag{41}$$

where $\Delta v = v - v_0$. The enthalpy equation of state can be obtained by substituting Eqs. (41) and (38) into Eq. (6), yielding

$$\boxed{h\,(T, v) = h_0 + C_v\,\Delta T + \frac{\beta}{\chi}(T\, v - T_0\, v_0) - \frac{\Delta v}{\chi}\;.} \tag{42}$$

[1] Using the formula $\int \ln x = x\,\ln x - x$.

where $h_0 = e_0 + p_0\, v_0$.

For code implementation it is useful to deduce expressions for $\rho(T,p)$, $h(T,p)$ and their derivatives. An expression for the density can be deduced directly from Eq. (34)

$$\boxed{\rho\,(T,p) = \rho_0\, \exp\left[\,-\beta\,(T-T_0) + \chi\,(p-p_0)\,\right]} \tag{43}$$

From definitions (8) and (9) it follows

$$\left(\frac{\partial\,\rho}{\partial\,T}\right)_p = -\beta\,\rho \qquad \text{and} \qquad \left(\frac{\partial\,\rho}{\partial\,p}\right)_T = \chi\,\rho \tag{44}$$

The expression for $h(T,p)$ can be found integrating Eq. (26). Using Eq. (34) one has

$$\left(\frac{\partial\,h}{\partial\,T}\right)_p = C_p \tag{45}$$

$$\left(\frac{\partial\,h}{\partial\,p}\right)_T = \frac{1-\beta\,T}{\rho_0} \exp[\beta(T-T_0) - \chi(p-p_0)] \tag{46}$$

which can be integrated using Eq. (29), yielding

$$h\,(T,p) = h_0 + \int_{T_0}^{T} C_p\, dT + \frac{1-\beta\,T}{\rho_0\,\chi} \exp[\beta(T-T_0)]\{\exp[-\chi(p-p_0)] - 1\} \tag{47}$$

where $h_0 = h(T_0, p_0)$.

2.7 Physical properties and equations of state for the Pb-Bi eutectic

The set of Lead-Bismuth reference physical properties, used for computation purposes by the EADF working group, is listed in Tab. 1. These data are based on the information found in the literature [6]. For each property a recommended correlation as a function of temperature was identified, valid in the application range of the EADF ($150°C < T < 700°C$). It is useful for

Property	Unit	Relationship
Density	$\frac{Kg}{m^3}$	$\rho = 10737 - 1.375\,T$
Specific heat at constant pressure	$\frac{J}{Kg\,°C}$	$C_p = 146.5$
Vapour pressure	Pa	$P_v = \exp\left[40.304 - 26.474\,\ln T + 3.044(\ln T)^2\right]$
Saturation temperature	$°C$	$T_{sat} = \exp\left[6.766 + 0.07473\,\ln p + 0.001541(\ln p)^2\right]$
Thermal conductivity	$\frac{W}{m\,°C}$	$k = 7.26 + 0.0123\,T$
Dynamic viscosity	$\frac{Kg}{m\,s}$	$\mu = 3.26 \times 10^{-3} - 6.26 \times 10^{-6}\,T + 4.63 \times 10^{-9}\,T^2$

Table 1: : Lead-Bismuth physical properties. The temperature values in the relationships are expressed in $°C$, pressures are in Pa.

the following consideration to estimate the range of variation of the thermodynamic variables in the EADF. Tab. 2 shows the order of magnitude of temperature, temperature variation, pressure and pressure variations in the EADF. The most significant pressure variations are due to the hydrostatic load: the reported Δp is referred to a height of 10 m. The relationship $\rho(T)$ in Tab.

Quantity	Unit	Estimated value
T	K	800
ΔT	K or ($°C$)	200
p	Pa	10^5
Δp	Pa	10^6

Table 2: : Order of magnitude of thermodynamic variables in the EADF.

1 is the first equation of state for the Pb-Bi. It can be deduced by integrating Eq. (15) with the hypothesis

$$\beta\,\rho = c_{\rho T} \equiv \text{const} \tag{48}$$
$$\chi\,\rho = c_{\rho p} \equiv \text{const} \tag{49}$$

yielding

$$\Delta\rho = \rho(-\beta\,\Delta T + \chi\,\Delta p) \quad . \tag{50}$$

Considering that $\beta \simeq 10^{-4}\,K^{-1}$ and $\chi \simeq 3 \times 10^{-11}\,Pa^{-1}$ and using the values in Tab. 2, we have

$$\beta\,\Delta T \simeq 10^{-2}$$
$$\chi\,\Delta p \simeq 10^{-5}$$

so the assumption

$$\chi\,\Delta p \ll \beta\,\Delta T$$

is justified and the final expression for the first equation of state for the Pb-Bi becomes

$$\rho(T) = \rho_0 - c_{\rho T}\,(T - T_0) \quad . \tag{51}$$

Taking $T_0 = 0\,°C$ we have

$$\boxed{\rho(T) = \rho_0 - c_{\rho T}\,T} \tag{52}$$

where $c_{\rho T} = 1.375\ Kg/m^3/K$ and $\rho_0 = 10737\ Kg/m^3$ if T is expressed in $°C$ and $\rho_0 = 11112\ Kg/m^3$ if T is in K.

Taking into account Eq. (48), from Eq. (23) it follows

$$\left(\frac{\partial C_p}{\partial p}\right)_T = -\frac{2\,c_{\rho T}^2\,T}{\rho^3} \quad .$$

The above quantity is order 10^{-9} which implies, for a $\Delta p = 10^6\ Pa$, a variation of the C_p of order 10^{-3} (i.e. 0.001 %). This justify the assumption of considering C_p independent of pressure. The further assumption of C_p independent of temperature is also congruent with the thermodynamic model. Therefore

$$C_p \equiv const\ . \tag{53}$$

The above assumptions imply that C_v is not constant. In fact, from Eq. (12), (48) and (49) it follows

$$C_v = C_p - \frac{c_{\rho T}^2\,T}{c_{\rho p}\,\rho^2} \quad . \tag{54}$$

Considering for example two states at $T = 400\,K$ and $T = 800\,K$, using Tab. 1 and considering that $c_{\rho p} \simeq 3 \times 10^{-7}$, we have $C_v(400) = 124\,J/Kg/K$ and $C_v(800) = 96\,J/Kg/K$ corresponding to a variation of about 25 %.

The second equation of state, written in term of enthalpy as a function of T and p, can be easily found from Eqs. (26). We have

$$\left(\frac{\partial h}{\partial T}\right)_p = C_p$$

$$\left(\frac{\partial h}{\partial p}\right)_T = \frac{1}{\rho(T)}\left(1 - \frac{c_{\rho T}\,T}{\rho(T)}\right)$$

which, after integration and taking also in account Eq. (52), becomes

$$\boxed{h(T,p) = h_0 + C_p\,\Delta T + \frac{\Delta p}{\rho_0 - c_{\rho T}\,T}\left(1 - \frac{c_{\rho T}\,T}{\rho_0 - c_{\rho T}\,T}\right)\ .} \tag{55}$$

An analysis of the order of magnitude of the terms in Eq. (55), using the values in Tab. 1, shows that the pressure term contribution to enthalpy variations is order 0.4 % of the temperature term contribution. Therefore the further assumption

$$h = h(T) = h_0 + C_p\,\Delta T \tag{56}$$

can be accepted. This is the expression usually adopted for the enthalpy in the commercial CFD codes and corresponds to the hypothesis of thermally perfect fluid.

3 Phenomenology of Lead-Bismuth natural circulation

In this section a one dimensional thermo-fluid-dynamic analysis of the Lead-Bismuth natural circulation in the EADF will be done, in order to give prominence to the general physics of the problem.

Fig. 1 shows the general layout of the Energy Amplifier. In the conceptual design of the EA both the target and the primary cooling circuit work in natural circulation. In the EADF the natural circulation is enhanced through gas injection in the rising channels. In order to describe

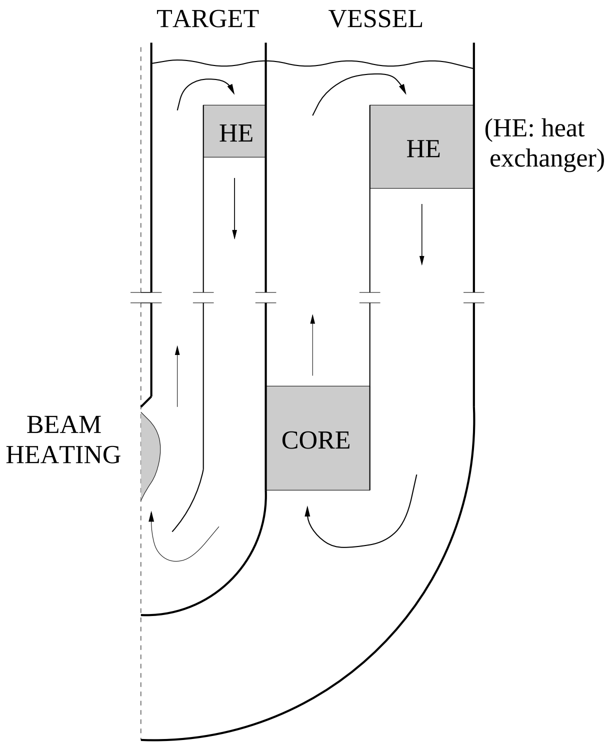

Figure 1: : EADF target and vessel.

the physics of the natural circulation, the one dimensional circuit shown in Fig. 2 is considered. The following assumption are considered:

1. the flow is stationary;
2. heat releases take place in the horizontal parts of the circuit;
3. dissipation losses in these parts are negligible with respect to the losses in the rest of the circuit;
4. the area A of the cross section of the circuit is constant.

These assumptions are not strictly necessary; the same general conclusions could be found without assumptions 2,3 and 4 (which are not verified in the EADF). However they simplify considerably the analytical treatment.

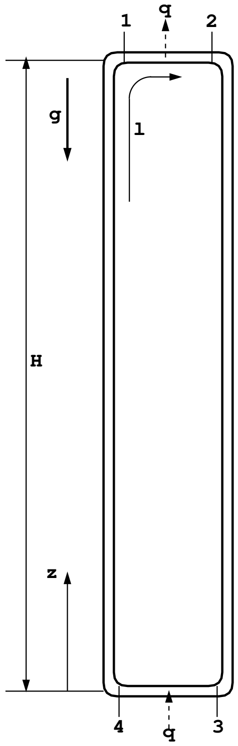

Figure 2: : One dimensional natural circulation circuit.

The flow in Fig. 2 can be described with the following set of equations (see App. B):

$$\dot{m} = \rho\, u\, A \equiv const \qquad \text{continuity equation} \tag{57}$$

$$\dot{m}\, \Delta u = -A\, \Delta p + \int_V \rho\, \mathbf{g} \cdot \mathbf{l}\, dV - F_\tau \qquad \text{momentum equation} \tag{58}$$

$$\Delta \left(e_k + \frac{p}{\rho} + g\, z \right) = -\int_{l_i}^{l_o} \frac{p}{\rho^2} \frac{d\rho}{dl}\, dl - \Phi \qquad \text{kinetic energy equation} \tag{59}$$

$$\Delta e = \int_{l_i}^{l_o} \frac{p}{\rho^2} \frac{d\rho}{dl}\, dl + \Phi + Q \qquad \text{internal energy equation} \tag{60}$$

$$\Delta(h + e_k + g\, z) = Q \qquad \text{enthalpy equation} \tag{61}$$

where V is the volume of the considered piece of circuit, l is duct curvilinear abscissa of versor $\mathbf{l}$, the subscripts i and o refer to the inlet and outlet sections respectively, $\dot{m}$ is the mass flow rate, $e_k = u^2/2$ is the kinetic energy, g the gravity acceleration, z a vertical coordinate (see Fig. 2), F_τ is the resultant of the viscous forces on the duct walls, Φ is the viscous dissipation in the control volume and Q is the heat transferred to the control volume. The momentum equation is valid in scalar form for a straight piece of duct. All the energy terms are per unit mass (J/Kg). Obviously, the three forms of the energy equation are not independent.

Eq (58) applied to the stretches 1-2 and 3-4 in Fig. 2 gives

$$\dot{m}\, \Delta u = -A\, \Delta p - F_\tau \quad . \tag{62}$$

From Eq. (57), we have

$$\dot{m}\,\Delta u = -\dot{m}\,u\frac{\Delta\rho}{\rho}$$

which in the EADF target, for example, ($\dot{m} \simeq 200\ Kg/s$, $u \simeq 1\ m/s$, $\Delta\rho/\rho \simeq 3\times 10^{-2}$) is about 6 Pa and can be neglected. For hypothesis 3, F_τ can be also neglected and Eq. (62) gives

$$p_2 - p_1 = p_4 - p_3 = 0 \quad . \tag{63}$$

i.e. the heat exchanges take place at constant pressure.

The application of Eq (58) to the stretch 2-3 yields

$$A\,(p_3 - p_2) = \rho_c\,g\,A\,H - F_\tau^{2-3}$$

or, writing $F_\tau/A = \Delta p_d$ (always positive),

$$p_3 = p_2 + \rho_c\,g\,H - \Delta p_d^{2-3} \tag{64}$$

where ρ_c is the fluid density in the cold column, which is almost constant. In analogous way, in the stretch 4-1 we obtain

$$p_1 = p_4 - \rho_h\,g\,H - \Delta p_d^{4-1} \quad . \tag{65}$$

From Eqs. (64), (65) and (63) it follows

$$\Delta p_d^{tot} = (\rho_c - \rho_h)\,g\,H = c_{\rho T}\,g\,H\,\Delta T \tag{66}$$

having used also Eq. (51). Eq. (66) is the classical equation for natural circulation loops, stating that the buoyancy pumping force is equilibrated by pressure losses in the circuit.

Eq (59), applied to the whole closed circuit, gives

$$-\int_{\text{circuit}} \frac{p}{\rho^2}\,d\rho = \Phi_{tot}$$

stating that the dissipation losses in the circuit are balanced by the expansion work ($p\,dv$). This work is performed were significant density variations occur, i.e. in the regions of heating (3-4) and cooling (1-2). Taking into account Eq. (65), we have

$$\Phi_{tot} = -p_1 \int_1^2 \frac{1}{\rho^2}\,d\rho - p_4 \int_3^4 \frac{1}{\rho^2}\,d\rho = (\rho_h\,g\,H + \Delta p_d^{4-1})\left(\frac{1}{\rho_h} - \frac{1}{\rho_c}\right)$$

Expressing the dissipation losses in terms of pressure losses as

$$\Phi_{tot} = \frac{\Delta p_d^{4-1}}{\rho_h} + \frac{\Delta p_d^{2-3}}{\rho_c}$$

Eq. (66) is found again. The energy transformations in the heating region can be explained by applying Eqs. (59), (60) and (61) to the stretch 3-4, yielding

$$\Delta\left(\frac{p}{\rho}\right) = -\int_3^4 \frac{p}{\rho^2}\,d\rho$$

$$\Delta e = \int_3^4 \frac{p}{\rho^2}\,d\rho + Q$$

$$\Delta(h) = Q$$

where the kinetic energy variation due to the density variation has been neglected (it can be easily shown that they are two orders of magnitude smaller than the pressure work). The second equation states that the heat Q given to the unit mass partly increases the internal energy and partly performs expansion work. The first equation states that this expansion work is used as pumping work ($d(p\,v)$) for the flow circulation, while the third equation just confirms that the enthalpy variation, i.e. the sum of internal energy variations and pumping work, is equal to the heat given to the flow.

In the stretch 4-1 we have

$$\begin{aligned}
&\Delta\left(\frac{p}{\rho} + gz\right) = \Phi^{4-1} \\
&\Delta e = \Phi^{4-1} \\
&\Delta(h) = -g\,H \quad .
\end{aligned}$$

Part of the pumping work is used for gaining potential energy, at the expense of static enthalpy, and partly is dissipated. The energy dissipated is re-converted into internal energy. An analogous reasoning holds in the stretch 2-3. The sum of the contributions of all parts of the circuit gives

$$\begin{aligned}
&\Delta e = 0 \\
&\Delta(h) = 0
\end{aligned}$$

as it is obvious for a close system with a zero net energy exchange.

In the case of the EADF, the expansion work is much smaller of the heat Q. For example, in the case of the target, given a heat release of $3 \times 10^4\ J/Kg$, from Eq. (55) we have $\Delta T \simeq 200K$. Assuming $\rho_c = \rho(500\,K)$, from Eq. (52) we find $\rho_c = 10425\,Kg/m^3$ and $\rho_h = 10150\,Kg/m^3$. Being $p_4 \simeq 10^6\ Pa$, the $p\,dv$ work is given by

$$\int_3^4 \frac{p}{\rho^2}\,d\rho = p_4\left(\frac{1}{\rho_h} - \frac{1}{\rho_c}\right) \simeq 2.6\,J/Kg$$

that is 0.01 % of the heat Q. As explained above, the energy dissipation Φ has the same order of magnitude of the $p\,vV$ work. Therefore, although necessary to explain the physics of the natural convection, the contributions of expansion work and dissipation on internal energy and enthalpy variations are negligible.

It should be noted that, for congruence, both the viscous dissipation and the expansion work terms should be neglected. For example, if just the viscous dissipation is canceled in Eq. (60), the $p\,dv$ term remains unbalanced and keeps on producing internal energy, never reaching a steady state[2]. However, in the case of the EADF, this term is small enough to be absorbed in the numerical error.

4 Conclusions

The thermodynamic model for the Pb-Bi flow in the Energy Amplifier Demonstration Facility was presented, in order to give some guidelines for the choice of the option to be used in the models for the numerical simulation of liquid metal flows. It was found that, in the case of the EADF, the enthalpy can be considered just a function of temperature.

[2] In the CFX commercial code, for example, the presence of the viscous term in the energy equation is optional.

The phenomenology of the natural circulation in the EADF was also presented, highlighting the energy exchange mechanisms in the different parts of the circuit. It was found that, although necessary to explain the physics of the phenomenon, the contributions of both the expansion work and the viscous dissipation can be neglected in the energy equation. In this case, the effect of natural circulation is present only in the momentum equation which is decoupled from the internal energy equation, that accounts just for the heat exchanges (see Eq. (60)).

A Thermodynamics Algebra

A.1 Mathematical theorems [4]

Let us consider the equation of state $\mathcal{F}(x, y, z) = 0$, where x, y and z are thermodynamic variables, Expliciting z we can write

$$dz = \left(\frac{\partial z}{\partial x}\right)_y dx + \left(\frac{\partial z}{\partial y}\right)_x dy = M\,dx + N\,dy \tag{67}$$

where

$$M = \left(\frac{\partial z}{\partial x}\right)_y \qquad \textit{and} \qquad N = \left(\frac{\partial z}{\partial y}\right)_x \tag{68}$$

If $z(x, y)$ is continuous with continuous derivatives, it must be

$$\boxed{\left(\frac{\partial M}{\partial y}\right)_x = \left(\frac{\partial N}{\partial x}\right)_y} \tag{69}$$

Eq. (69) is the necessary and sufficient condition for z to be a perfect differential form.

Two more useful theorems can be deduced as follows. We can write

$$dx = \left(\frac{\partial x}{\partial y}\right)_z dy + \left(\frac{\partial x}{\partial z}\right)_y dz \tag{70}$$

and

$$dy = \left(\frac{\partial y}{\partial z}\right)_x dz + \left(\frac{\partial y}{\partial x}\right)_z dx \tag{71}$$

Substituting the expression for dy from Eq. (71) in Eq. (70) we obtain

$$\left[\left(\frac{\partial x}{\partial y}\right)_z \left(\frac{\partial y}{\partial x}\right)_z - 1\right] dx + \left[\left(\frac{\partial x}{\partial y}\right)_z \left(\frac{\partial y}{\partial z}\right)_x + \left(\frac{\partial x}{\partial z}\right)_y\right] dz = 0 \tag{72}$$

which must be valid whatever the values of dx and dz, hence

$$\boxed{\left(\frac{\partial x}{\partial y}\right)_z = \left(\frac{\partial y}{\partial x}\right)_z^{-1}} \tag{73}$$

$$\boxed{\left(\frac{\partial x}{\partial z}\right)_y = -\left(\frac{\partial x}{\partial y}\right)_z \left(\frac{\partial y}{\partial z}\right)_x} \tag{74}$$

A.2 Maxwell equations

Applying Eq. (69) to the following thermodynamic differential forms:

$$\begin{aligned} de &= T\,ds - p\,dv \\ dh &= T\,ds + v\,dp \\ df &= -s\,dT - p\,dv \\ dg &= -s\,dT + v\,dp\,, \end{aligned}$$

where $f = e - T\,s$ is the Helmholtz' function and $g = h - T\,s$ is the Gibbs' function, the Maxwell equations can be obtained:

$$\left(\frac{\partial T}{\partial v}\right)_s = -\left(\frac{\partial p}{\partial s}\right)_v \tag{75}$$

$$\left(\frac{\partial T}{\partial p}\right)_s = \left(\frac{\partial v}{\partial s}\right)_p \tag{76}$$

$$\left(\frac{\partial p}{\partial T}\right)_v = \left(\frac{\partial s}{\partial v}\right)_T \tag{77}$$

$$\left(\frac{\partial v}{\partial T}\right)_p = -\left(\frac{\partial s}{\partial p}\right)_T \tag{78}$$

A.3 Entropy equations

Considering s as a function of T and v we can write

$$ds = \left(\frac{\partial s}{\partial T}\right)_v dT + \left(\frac{\partial s}{\partial v}\right)_T dv \tag{79}$$

Taking in account Eqs. (4) and (10) it follows

$$\left(\frac{\partial s}{\partial T}\right)_v = \frac{1}{T}\left(\frac{\delta Q}{\partial T}\right)_v = \frac{C_v}{T} \tag{80}$$

Using the Maxwell Eq. (77), theorem (74) and definitions (8) and (9) we can write

$$\left(\frac{\partial s}{\partial v}\right)_T = \left(\frac{\partial p}{\partial T}\right)_v = -\left(\frac{\partial p}{\partial v}\right)_T \left(\frac{\partial V}{\partial T}\right)_p = \frac{\beta}{\chi} \tag{81}$$

and finally

$$\boxed{ds = \frac{C_v}{T}\,dT + \frac{\beta}{\chi}\,dv} \tag{82}$$

In analogous way, writing s as a function of T and p we obtain

$$\boxed{ds = \frac{C_p}{T}\,dT - \beta\,v\,dp} \tag{83}$$

A.4 Specific heats equation

Subtraction of Eq. (82) form Eq. (83) yields

$$(C_p - C_v)\,dT = T\,\beta\left(\frac{1}{\chi}\,dv + v\,dp\right)$$

Dividing by dT and imposing $v \equiv$ cost. (or $p \equiv$ cost.) we obtain

$$(C_p - C_v) = \frac{\beta\,T}{\chi}\left(\frac{\partial v}{\partial T}\right)_p$$

and finally

$$\boxed{(C_p - C_v) = \frac{\beta^2\,T\,v}{\chi}} \tag{84}$$

A.5 Energy and enthalpy equations

Eq. (25) can be obtained from the differential form of e as a function of T and p

$$de = \left(\frac{\partial e}{\partial T}\right)_p dT + \left(\frac{\partial e}{\partial p}\right)_T dp.$$

Considering Eq. (3) and definition (9) we can write

$$\left(\frac{\partial e}{\partial T}\right)_p = \left(\frac{\delta Q}{\partial T}\right)_p - p\left(\frac{\partial v}{\partial T}\right)_p = C_p - \beta\, p\, v$$

Taking into account Eq. (5), Maxwell equation (78) and definitions (9) and (8) we obtain

$$\left(\frac{\partial e}{\partial p}\right)_T = T\left(\frac{\partial s}{\partial p}\right)_T - \left(\frac{\partial v}{\partial p}\right)_T = -T\left(\frac{\partial v}{\partial T}\right)_p - p\left(\frac{\partial v}{\partial p}\right)_T = -\beta\, T\, v + \chi\, p\, v$$

so yielding the final expression for de.

Eq. (27) can be obtained in a similar way, writing

$$dh = \left(\frac{\partial h}{\partial T}\right)_v dT + \left(\frac{\partial h}{\partial v}\right)_T dv.$$

Considering Eqs. (7), (10), (74), (8) and (9) we can write

$$\left(\frac{\partial h}{\partial T}\right)_v = \left(\frac{\delta Q}{\partial T}\right)_v + v\left(\frac{\partial p}{\partial T}\right)_v = C_v - v\left(\frac{\partial p}{\partial v}\right)_T\left(\frac{\partial v}{\partial T}\right)_p = C_v - \frac{\beta}{\chi}\, v$$

and, considering also Eq. (77),

$$\begin{aligned}\left(\frac{\partial h}{\partial v}\right)_T &= T\left(\frac{\partial s}{\partial v}\right)_T + v\left(\frac{\partial p}{\partial v}\right)_T = T\left(\frac{\partial p}{\partial T}\right)_v - \frac{1}{\chi} = -T\left(\frac{\partial p}{\partial v}\right)_T\left(\frac{\partial v}{\partial T}\right)_p - \frac{1}{\chi}\\ &= \frac{1}{\chi}(\beta\, T - 1)\end{aligned}$$

B Fluid-dynamic Governing Equations

The stationary continuity, momentum and energy equations are given respectively by [5]

$$\nabla\cdot\rho\,\mathbf{u} = 0 \tag{85}$$

$$\nabla\cdot\rho\,\mathbf{u}\,\mathbf{u} = -\nabla\, p + \nabla\cdot\tau + \rho\,\mathbf{g} \tag{86}$$

$$\nabla\cdot\rho\,\mathbf{u}\,E = \nabla\cdot(-p\,\mathbf{u} + \tau\cdot\mathbf{u} + \mathbf{q}) + \rho\,\mathbf{u}\cdot\mathbf{g} \tag{87}$$

where $\mathbf{u}$ is the velocity vector, $\mathbf{g}$ the gravity acceleration vector, $\mathbf{q} = k\,\nabla\, T$ the heat flux vector ($k \equiv$ thermal conductivity),

$$E = e + e_k \tag{88}$$

the total energy, being $e_k = V^2/2 = \mathbf{u}\cdot\mathbf{u}/2$ the kinetic energy, and τ is the stress tensor.

The equation for the kinetic energy e_k is obtained by multiplying Eq. (86) by $\mathbf{u}$, yielding

$$\nabla \cdot (\rho\, \mathbf{u}\, e_k) = -\nabla \cdot (p\, \mathbf{u}) + \nabla \cdot (\tau \cdot \mathbf{u}) + p\, \nabla \cdot \mathbf{u} + \rho\, \mathbf{u} \cdot \mathbf{g} - \phi\,. \tag{89}$$

where the viscous dissipation ϕ is defined as

$$\phi = \tau : \nabla\, \mathbf{u}\,. \tag{90}$$

and is always positive. The gravity vector can be written as

$$\mathbf{g} = -\nabla G$$

where G is the gravity potential which, if z is a vertical direction opposite to the gravity vector, is given by

$$G = g\, z \tag{91}$$

Therefore, using also Eq. (85), we can write

$$\rho\, \mathbf{u} \cdot \mathbf{g} = \rho\, \mathbf{u} \cdot \nabla G = \nabla \cdot (\rho\, \mathbf{u} G) \tag{92}$$

and Eq. (89) can be written as

$$\nabla \cdot [\rho\, \mathbf{u}\, (e_k + \frac{p}{\rho} + g\, z)] = \nabla \cdot (\tau \cdot \mathbf{u}) + p\, \nabla \cdot \mathbf{u} - \phi \tag{93}$$

having used the relation

$$\nabla \cdot (p\, \mathbf{u}) = \nabla \cdot (\rho\, \mathbf{u}\, \frac{p}{\rho}) = \rho\, \mathbf{u} \cdot \nabla(\frac{p}{\rho})\,.$$

The internal energy equation can be obtained by subtracting Eq. (89) from Eq. (87), yielding

$$\nabla \cdot (\rho\, \mathbf{u}\, e) = -p\, \nabla \cdot \mathbf{u} + \phi + \nabla \cdot \mathbf{q} \tag{94}$$

Eq. (87) can be written in terms of enthalpy by using Eqs. (6), (92) and (85), yielding

$$\nabla \cdot [\rho\, \mathbf{u}\, (h + e_k + g\, z)] = \nabla \cdot (\tau \cdot \mathbf{u}) + \nabla \cdot \mathbf{q} \tag{95}$$

The one dimensional form of Eqs. (85), (86), (93), (94) and (95) can be obtained through the integration of the above equations over a control volume V given by a piece of duct of cross section area A. Using the Gauss theorem with little algebra we obtain

$$\dot{m} = \rho\, u\, A \equiv const \tag{96}$$

$$\dot{m}\, \Delta \mathbf{u} = -\Delta(p\, A\, \mathbf{I}) + \int_V \rho\, \mathbf{g}\, dV + \mathbf{F}_p - \mathbf{F}_\tau \tag{97}$$

$$\Delta(e_k + \frac{p}{\rho} + g\, z) = -\int_{l_i}^{l_o} \frac{p}{\rho^2} \frac{d\rho}{dl}\, dl - \Phi \tag{98}$$

$$\Delta e = \int_{l_i}^{l_o} \frac{p}{\rho^2} \frac{d\rho}{dl}\, dl + \Phi + Q \tag{99}$$

$$\Delta(h + e_k + g\, z) = Q \tag{100}$$

where Δ refers to the difference between the value in the outlet (subscript o) and the inlet (subscript i) sections, l is duct curvilinear abscissa of versor $\mathbf{l}$, u is the velocity module, $\dot{m}$ is the mass flow rate,

$$\mathbf{F}_p = \int_{S_l} p\,\mathbf{n}\,dS$$

is the resultant of the pressure forces applied to the duct surface S_l,

$$\mathbf{F}_\tau = \int_{S_l} \tau_w\,\mathbf{l}\,dS$$

is the resultant of the viscous forces applied to the duct surface S_l,

$$\Phi = \frac{1}{\dot{m}} \int_V \phi\,dV \qquad [J/Kg]$$

is the total dissipation per unit mass in the control volume and

$$Q = \frac{1}{\dot{m}} \int_{S(V)} q\,dS \qquad [J/Kg]$$

is the total heat given to the control volume.

The term

$$\int_V \nabla \cdot (\tau \cdot \mathbf{u})\,dV = \int_{S(V)} (\tau \cdot \mathbf{u}) \cdot \mathbf{dS} \simeq 0$$

represents an the work done by viscous stresses and is zero on all the solid walls (u = 0) and can be neglected in the inlet and outlet sections (the normal component of the stress tensor are usually small). Also, the following relation was used

$$\int_V p\,\nabla \cdot \mathbf{u}\,dV = -\int_V \frac{p}{\rho}\mathbf{u} \cdot \nabla\rho\,dV = -\int_V \rho\,u\frac{p}{\rho^2}\frac{d\rho}{dl}\,A\,dl = -\dot{m}\int_V \frac{p}{\rho^2}\,d\rho = \dot{m}\int_V p\,dv \qquad .$$

For a straight duct, the momentum equation (Eq (97))becomes

$$\dot{m}\,\Delta u = -\Delta(p\,A) + \int_V \rho\,\mathbf{g} \cdot \mathbf{l}\,dV - F_\tau \tag{101}$$

being $\mathbf{F}_p = 0$.

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