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D TARZIA

Analysis of a bibliography on moving and free boundary problems for the heat equation. Some results for the one-dimensional Stefan problem using the Lame–Clapeyron and Neumann solutions

This paper is made up of two parts which are independent of each other. The first is concerned with a bibliographical analysis of a wide collection of papers which are of interest ot this International Symposium. The second is concerned with the different results obtained by using the explicit solutions in the one-dimensional Stefan problem.

1. AN ANALYSIS OF A BIBLIOGRAPHY ON MOVING AND FREE BOUNDARY PROBLEMS FOR THE HEAT EQUATION. THE STEFAN PROBLEM

A review of a long bibliography on moving and free boundary problems of the heat equation, particularly regarding the Stefan problem, is presented in [71]. The bibliography is analysed and classified into theoretical, numerical and experimental papers and also those concerning possible applications. The plan developed in [71] is the following:

I. Moving boundary problems for the heat equation

I.1. One-dimensional case

I.2. Multidimensional case

I.3. Physical applications

I.4. Applications to free boundary problems

II. Free boundary problems for the heat equation

II.1. Free boundary problems of Stefan type

II.1.1. One-dimensional case

II.1.1.1. One-phase problem (theoretical, numerical methods and applications)

II.1.1.2. Two-phase problem (theoretical, numerical methods and applications)

II.1.2 Multidimensional case

II.1.2.1. One-phase problem (theoretical, numerical methods and applications)

II.1.2.2. Two-phase problem (theoretical, numerical methods and applications)

II.1.3. Other generalities

II.1.3.1. Free boundary problems in a gaseous state

II.1.3.2. Experimental works
II.1.3.3 Solid-liquid interphase
II.1.3.4 Other applications
II.2. Free boundary problems not of Stefan type
II.2.1. Diffusion-consumption of oxygen in absorbing tissue
II.2.2. Flow of two immiscible fluids in a porous medium
II.2.3. Movement of a compressible fluid through a porous medium
II.2.4. Impact of a viscoplastic bar on a rigid obstacle
II.2.5 Chemical reactions between two substances
II.2.6 Other free boundary problems for the heat equation
II.2.6.1 Of an implicit type
II.2.6.2 Of an explicit type.

To avoid confusion between the terms "free boundary" and "moving boundary", I think it is advisable to point out the difference between them, especially since both terms are used indiscriminately in the English literature (see, e.g., the previous International Symposium on this subject [1, 29, 51, 54, 85]. On the other hand, in [18] the author discusses the relationship between moving boundary problems (parabolic and time-dependent) and free boundary problems (elliptic and steady state). Because of this definition, approximately 1% of the references in the long bibliography on free boundary problems [17] are concerned with heat conduction and diffusion [17, §1.6] (there exist only 53 references). Our definition follows the one used in the Italian literature (Florence group). In general, the problems given for the heat or diffusion equation are classified in the following way:

- boundary problems
  - fixed
  - moving
  - free
    - implicit type
    - explicit type

The fixed boundary problems for the heat equation are those studied in the domain $(x_1,x_2) \times (0,T)$, i.e., the classical problems analysed in any basic course of partial differential equations, such as:

$$
(\mathrm{FBP})\begin{cases}
u_t - u_{xx} = f(x,t), & x_1 < x < x_2, \quad 0 < t < T \\
u(x,0) = h(x), & x_1 < x < x_2 \\
u(x_1,t) = f_1(t) \text{ or } & u_x(x_1,t) = f_1(t), \quad 0 < t < T \\
u(x_2,t) = f_2(t) \text{ or } & u_x(x_2,t) = f_2(t), \quad 0 < t < T
\end{cases}
$$

which are not included in our analysis and classification.

The moving boundary problems for the heat equation are those studied in the domain $\{(x,t)/s_1(t) < x < s_2(t),\ 0 < t < T\}$ with $s_1(t) < s_2(t)$, functions given in $(0,T)$, i.e., the spatial domain of the unknown function varies with time because of a law of movement, known *a priori*, such as

$$\text{(MBP)}\quad \begin{cases} u_t - u_{xx} = f(x,t), & s_1(t) < x < s_2(t),\ \ 0 < t < T \\ u(x,0) = h(x), & s_1(0) < x < s_2(0) \\ u(s_1(t),t) = f_1(t) \text{ or } u_x(s_1(t),t) = f_1(t), & 0 < t < T \\ u(s_2(t),t) = f_2(t) \text{ or } u_x(s_2(t),t) = f_2(t), & 0 < t < T. \end{cases}$$

Moreover, the domain can be of the form $\{(x,t)/x < s(t),\ 0 < t < T\}$ or $\{(x,t)/s(t) < x,\ 0 < t < T\}$. All these problems were originally studied in [6,22,34,35,38-40,44] and in the last decade in [26-28].

The free boundary problems for the heat equation are those in which the spatial domain of the unknown function varies with time because of a law of movement not known *a priori*. The fact of not knowing the boundary or part of it, determines, of course, the mathematical need to impose new conditions on the unknown functions, which will depend on the physical problem studied. In general, the new condition to be imposed on the unknown function is deduced from the principle of conservation of energy through the boundary. Thus it follows that this boundary is the complementary unknown of the problem, and is called the free boundary of the problem under analysis.

Therefore, the essential difference between the moving and free boundary problems lies in the fact of the existence of a boundary whose law of movement is known in the first case and unknown in the second, the latter being another unknown of the problem itself.

The free boundary problems for the heat equation are divided into two classes, the explicit and the implicit types, according to whether the speed of the free boundary appears explicitly, in the conditions imposed on this boundary. That is to say, if the free boundary is given by $s = s(t)$, then the problem will be of an explicit (implicit) type if $\dot{s}(t)$ appears (does not appear) in the condition imposed for $x = s(t)$. An example of a free boundary problem of explicit type is the classical Stefan problem [9, 11 (Ch. 11), 15 (Ch. 13), 19, 23, 30 (Ch. 8), 49 (Ch. 8-10), 55 (Ch.10), 59] and of one of implicit type is the diffusion-consumption of oxygen in a living tissue [16, 45]. In general, free boundary problems of explicit and implicit types are related to each other [25, 61].

To finish this part, it is important to point out that the subject has been reviewed in many papers. These include, apart from those already mentioned, [3,7,50,57,58,62]. A bibliography on moving free boundary problems with key word index is given in [86]. At the moment, we are compiling a bibliography with more than 1700 references on this subject.

2. SOME RESULTS FOR THE ONE-DIMENSIONAL STEFAN PROBLEM USING THE LAME-CLAPEYRON AND NEUMANN SOLUTIONS

Different results using the explicit solutions in the one-phase or two-phase Stefan problem have been obtained, for example, in the following problems:

(i) Relationship between the similarity and inmobilization of domain methods [60].
(ii) Density jump at the free boundary [11, 13, 14, 59].
(iii) Coupling of temperature and concentration [59, 64, 78, 84].
(iv) Solidification of alloys [75, 76, 81].
(v) Composite body with simultaneous solidification and melting [24].
(vi) Existence of multiphases [59, 80, 82, 83].
(vii) Phase-change heat and mass transfer process in a porous medium [12, 46-48, 52, 53].
(viii) Oxidation of zirconium [20, 21 (interaction between UO_2 and Z_r)].
(ix) Absorption of a gas (oxygen) by a solid [31].
(x) with variable thermal coefficients [13, 77].
(xi) Solidifcation with mushy zone [63].

We present here some results connected with one-dimensional one-phase and two-phase Stefan problems, which are obtained by using the Lame-Clapeyron [43] and Neumann [7,11,79] solutions, for example: inequality for the heat flux on the fixed face for obtaining a phase-change process with a density jump, inequalities for the coefficient that characterizes the free boundary, determination of one or two thermal coefficients through a phase-change experiment (and also including the mushy region model given by Solomon-Wilson-Alexiades), determination of thermal coefficients through approximate methods (Stefan's quasi-stationary method, Goodman's integral balance method, Biot's variational method) and its comparison with those given through the analytical solution. Therefore, we shall consider several different problems with their corresponding results (we shall assume from now on and without loss of generality, that the material phase-change temperature is 0°C).

2.1 An inequality for the heat flux on a fixed face of a one-dimensional finite material undergoing a steady-state phase-change problem

Problem P1 We have a one-dimensional material of finite length $x_0 > 0$, represented by the interval $(0,x_0)$, and we consider the steady-state heat conduction problem with the following boundary condition: on the face $x = 0$ we have a temperature $B > 0$ and on the face $x = x_0$ we have an outward heat flux $q > 0$. The material loses energy through the face $x = x_0$, therefore its temperature will be below the value B; but, in general, the material will not undergo a phase change. Which inequality should verify the heat flux q for the material to undergo a phase change within?

We have the following results:

Property 1 [68] (i) The material will undergo a phase-change within iff $q > k_2 B/x_0$. Moreover, in such a case the free boundary $s \in (0,x_0)$ and the temeprature $\theta = \theta(x)$ are given by

$$\theta(x) = \begin{cases} B(1 - \frac{x}{s}) \text{ if } 0 < x < s, & s = \frac{k_2 B}{q} \\ -\frac{k_2 B}{k_1}(\frac{x}{s} - 1) \text{ if } s < x < x_0. & \end{cases} \tag{1}$$

(ii) If $q < k_2 B/x_0$, then we have a steady heat conduction problem only for the liquid phase.

(iii) If there exists an energy consumption $g = g(x) < 0$ within the material, then it will undergo a phase change iff q verifies the following inequality:

$$q > \frac{k_2 B}{x_0} + \frac{1}{x_0}\int_0^{x_0} t\, g(t)dt. \tag{2}$$

Moreover, the free boundary is the only element $s \in (0,x_0)$ which satisfies the equation $u(s) = 0$, where

$$u(x) = k_2 B + \left(\int_0^{x_0} g(t)dt - q\right)x - \int_0^x (x-t)g(t)dt. \tag{3}$$

2.2. An inequality for the heat flux on the fixed face $x = 0$ of a semi-infinite material (initially at uniform temperature) for it to undergo an evolution phase-change problem

Problem P2 We have a semi-infinite material in solid phase at constant temperature $-C < 0$. If on the fixed face $x = 0$ we impose a heat flux of the form $q(t) = -q_o/\sqrt{t}$ ($q_o > 0$) at $t > 0$, we may ask for which values of q_o will the material undergo a phase change?

We have the following results:

Property 2 [2, 64, 69] (i) If we consider the density jump at the free boundary, i.e., $\rho_1 \neq \rho_2$, then the material will undergo a phase change within, iff q_o verifies the inequality

$$q_o > \frac{Ck_1}{a_1\sqrt{\pi}} = C\left(\frac{\rho_1 c_1 k_1}{\pi}\right)^{\frac{1}{2}} \tag{4}$$

Moreover, in such case, the free boundary $s = s(t)$ and the temperatures $\theta_2 = \theta_2(x,t)$ and $\theta_1 = \theta_1(x,t)$ of the liquid and solid phases, respectively, are given by

$$\theta_1(x,t) = \frac{-C}{\operatorname{erfc}(w/a_o)}\left[\operatorname{erf}\left(m_1 + \frac{x}{2a_1\sqrt{t}}\right) - \operatorname{erf}\left(\frac{w}{a_o}\right)\right],\ x > s(t),\ t > 0$$

$$\theta_2(x,t) = \frac{a_2 q_o\sqrt{\pi}}{k_2}\left[\operatorname{erf}\left(\frac{w}{a_2}\right) - \operatorname{erf}\left(\frac{x}{2a_2\sqrt{t}}\right)\right],\ 0 < x < s(t),\ t > 0 \tag{5}$$

$$s(t) = 2w\sqrt{t}, \qquad m_1 = \frac{|\varepsilon| w}{a_1},\quad a_0 = \frac{a_1}{1+|\varepsilon|},\quad \varepsilon = \frac{\rho_2-\rho_1}{\rho_1}$$

where $w > 0$ is the unique solution of the equation

$$F_o(x) = x,\ x > 0 \tag{6}$$

with

$$F_o(x) = \frac{q_o}{\ell\rho_2}\exp\left(-\frac{x^2}{a_2^2}\right) - \frac{C\,k_1}{\ell\rho_2 a_1\sqrt{\pi}}\,\frac{\exp(-x^2/a_o^2)}{\operatorname{erfc}(x/a_o)}\,. \tag{7}$$

(ii) If $q_o < Ck_1/a_1\sqrt{\pi}$, there is no solution for the fusion problem P2; we just have a heat conduction problem in the initial solid phase.

2.3 Inequalities for the coefficient σ of the free boundary $s(t) = 2\sigma\sqrt{t}$ of the Neumann solution for the two-phase Stefan problem

Since the solution (5) of (P2) verifies the condition $B_o = \theta_2(0,t) = a_2 h_o \sqrt{\pi}\, f(w/a_2)/k_2 > 0$, we can consider the Neumann problem (on $x = 0$ the semi-infinite material has a temperature $B > 0$) whose solution is given by

$$\theta_1(x,t) = \frac{-C}{\operatorname{erfc}(\sigma/a_o)} \left[\operatorname{erf}\left(\delta_1 + \frac{x}{2a_1\sqrt{t}}\right) - \operatorname{erf}\left(\frac{\sigma}{a_o}\right)\right], \quad x > s(t), \; t > 0$$

$$\theta_2(x,t) = B\left[1 - \frac{\operatorname{erf}\left(\frac{x}{2a_2\sqrt{t}}\right)}{\operatorname{erf}\left(\frac{\sigma}{a_2}\right)}\right], \quad 0 < x < s(t), \; t > 0 \tag{8}$$

$$s(t) = 2\sigma\sqrt{t}, \quad \delta_1 = \frac{|\varepsilon|\sigma}{a_1}$$

where $\sigma > 0$ is the unique solution of the equation

$$F(x) = x, \quad x > 0 \tag{9}$$

where

$$F(x) = \frac{Bk_2}{\ell\rho_2 a_2\sqrt{\pi}} \frac{\exp(-x^2/a_2^2)}{\operatorname{erf}(x/a_2)} - \frac{Ck_1}{\ell\rho_2 a_1\sqrt{\pi}} \frac{\exp(-x^2/a_o^2)}{\operatorname{erfc}(x/a_o)} . \tag{10}$$

Then, we obtain the following properties

Property 3 [2] If inequality (4) is valid and we connect (P2) with Neumann's, taking $B = B_o$, then we obtain

(a) $\sigma = w$ (therefore the two problems are equivalent).

(b) The coefficient σ, which characterizes the free boundary of Neumann's solution, satisfies the inequality

$$\operatorname{erf}\left(\frac{\sigma}{a_2}\right) < \frac{B}{C}\left(\frac{k_2\rho_2 c_2}{k_1\rho_1 c_1}\right)^{\frac{1}{2}}. \tag{11}$$

Property 4 [65] For the case $\rho_1 = \rho_2$, the coefficient σ of solution (8) satisfies numerous inequalities, for example:

$$\text{(i)} \quad \sigma < a_2 \, J^{-1}\left(\frac{Bc_2}{(\ell + Cc_1)\sqrt{\pi}}\right)$$

$$\text{(ii)} \quad \sigma < a_2 \, Y^{-1}\left(\frac{Bc_2}{\ell\sqrt{\pi}}\right) \tag{12}$$

with $J(x) = x \operatorname{erf}(x)$, $Y(x) = J(x) + \dfrac{Ck_1}{\rho\ell a_2 a_1\sqrt{\pi}} \dfrac{\operatorname{erf}(x)\exp\left(-\frac{a_2^2}{a_1^2}x^2\right)}{\operatorname{erfc}\left(\frac{a_2}{a_1}x\right)}$

which are properties that hold for all materials.

2.4 Determination of one or two thermal coefficients of a semi-infinite material through a one-phase Lame-Clapeyron problem with an overspecified condition on the fixed face

Let us suppose that one or two of the four coefficients k,ℓ,c,ρ of a phase (e.g., liquid) of some given semi-infinite material are unknown. If, by means of a phase-change experiment (fusion of the material at its melting temperature) we are able to measure certain quantities, then we shall be able to find formulas for the determination of the unknown coefficients. We shall consider a (direct or inverse) one-phase Lame-Clapeyron problem (or one-phase Stefan problem with constant thermal coefficients) [43] with an overspecified condition on the fixed face $x = 0$. This overspecified condition consists of the specification of the heat flux through the fixed face of the material undergoing the phase-change process. Other boundary value problems for the one-dimensional heat equation with an overspecified condition on a part of the boundary have been analysed [9,10,41,42] (see also the numerous references in [72] on the determination of thermal coefficients).

Problem P3 (Determination of one unknown thermal coefficient). We shall find the function $s = s(t) > 0$ (free boundary), defined for $t > 0$ with $s(0) = 0$; the temperature $\theta = \theta(x,t)$ of the liquid phase, defined for $0 < x < s(t)$, $t > 0$, and one of the four coefficients k,ℓ,c,ρ of the phase-change material so that they satisfy the following conditions:

$$
\begin{aligned}
&\text{(i)} \quad \theta_t = a^2\theta_{xx}, \quad 0 < x < s(t), \quad t > 0 \\
&\text{(ii)} \quad \theta(s(t),t) = 0, \quad t > 0 \\
&\text{(iii)} \quad -k\theta_x(s(t),t) = \rho\ell\dot{s}(t), \quad t > 0 \\
&\text{(iv)} \quad s(0) = 0 \\
&\text{(v)} \quad \theta(0,t) = \theta_0 > 0, \quad t > 0 \\
&\text{(vi)} \quad k\theta_x(0,t) = -\frac{h_0}{\sqrt{t}} \quad (h_0 > 0), \quad t > 0
\end{aligned}
\tag{13}
$$

where $h_0 > 0$ characterizes the heat flux on the fixed face $x = 0$. We have

Property 5 If the coefficients $\theta_0 > 0$ and $h_0 > 0$ are given from experience of a phase-change material, the results for the four possible cases are given in [70]. For example, if the data verifies the condition

$$\frac{\theta_0}{h_0}\left(\frac{k\rho c}{\pi}\right)^{\frac{1}{2}} < 1 \tag{14}$$

then the coefficient ℓ is determined by

$$\ell = h_0\left(\frac{c}{\rho k}\right)^{\frac{1}{2}} \frac{\exp(-\xi^2)}{\xi} \tag{15}$$

where $\xi > 0$ is the unique solution of the equation

$$\operatorname{erf}(x) = \frac{\theta_0}{h_0}\left(\frac{k\rho c}{\pi}\right)^{\frac{1}{2}}, \quad x > 0. \tag{16}$$

Problem P4 (Determination of two unknown thermal coefficients) If we assume that the moving boundary is given by $s(t) = 2\sigma\sqrt{t}$, with $\sigma > 0$, the problem is reduced to finding the temperature $\theta = \theta(x,t)$ of the liquid phase, defined for $0 < x < s(t)$, $t > 0$, and two of the four coefficients k,ℓ,c,ρ such that they satisfy the conditions (13 (i) - (iii), (v), (vi)). We have

Property 6 If the coefficients $\theta_0 > 0$, $h_0 > 0$ and $\sigma > 0$ are determined from experience of a phase-change material, the results for the six possible cases are given in [72]. For example, for any data the simultaneous determination of the coefficients k,ℓ is given by

$$\ell = \frac{h_0}{\rho\sigma} \exp(-\xi^2), \quad k = \frac{\rho c \sigma^2}{\xi^2} \tag{17}$$

where $\xi > 0$ is the unique solution of the equation

$$J(x) = \frac{\rho c \sigma \theta_0}{h_0 \sqrt{\pi}}, \; x > 0. \tag{18}$$

When the coefficient k is unknown, a new variant for the simultaneous calculation of some of the thermal coefficients of a semi-infinite material can be stated.

Problem P5 This is the same problem P3 or P4 but now considering problem (13) with the overspecified condition

(13vi bis) $\theta_x(0,t) = \frac{-H_0}{\sqrt{t}}, \; t > 0 \quad (H_0 > 0)$

instead of (13vi), in which the thermal conductivity k does not appear. The coefficient H_0 characterizes the temperature gradient on the fixed face $x = 0$ and may be determined experimentally.

REMARK 1 The results corresponding to problem P5 are given in [73].

REMARK 2 To calculate the coefficient H_0, we need the experimental determination of the temperature gradient on the fixed face $x = 0$ with the Condition (13v) of constant temperature. On the other hand, according to Problem P3 or P4 we need the experimental determination of the heat flux in $x = 0$ to calculate the coefficient h_0. It is held that this new variant may, to some extent, simplify the experimental results required for the application of the method.

Note that if the coefficient k is known, then the idea of problem P5 coincides with that in problems P3 or P4, through the relation $h_0 = kH_0$.

REMARK 3 A generalization of problems P3 and P4 through a two-phase Stefan problem is given in [65], with six cases for the determination of one unknown thermal coefficient and fifteen for the simultaneous determination of two unknown thermal coefficients.

2.5 Determination of unknown thermal coefficients of a semi-infinite material through the Solomon-Wilson-Alexiades model of a mushy region for the one-phase Lame-Clapeyron problem with an overspecified condition on the fixed face

We consider a semi-infinite material that is initially assumed to be solid at its melting temperature 0°C. At time $t = 0$, a constant temperature $\theta_0 > 0$ is imposed at $x = 0$ and then fusion ensues, in which three distinct regions can be distinguished [63]:

(H1) Solid, at temperature 0°C, occupying the region $x > r(t)$

(H2) Liquid, at temperature $\theta(x,t) > 0$, occupying the region $0 < x < s(t)$, where $s(t) < r(t)$.

(H3) Mushy region, at temperature $\theta(x,t) \equiv 0$, occupying the region $s(t) < x < r(t)$. Thus, the mushy region is taken to be isothermal, and we make the following two assumptions on this structure:

(i) the material contains a fixed fraction $\varepsilon\ell (0 < \varepsilon < 1)$ of the total latent heat ℓ, that is,

$$-k\, \theta_x(s(t),t) = \rho\ell[(1-\varepsilon)\dot{s}(t) + \varepsilon\dot{r}(t)],\ t > 0. \tag{19}$$

(ii) its width is inversely proportional to the temperature gradient, that is,

$$-\theta_x(s(t),t)(r(t)-s(t)) = \gamma > 0,\ t > 0. \tag{20}$$

Problem P6 This is the same problem P3 or P4 or P5, but now considering the conditions (13i-ii-v), (13vi) or (13vibis), (19), (20) and $s(0) = r(0) = 0$. We have

Property 7 The results corresponding to problem P6 are given in [74]. For example, if the data verify the conditions

$$\begin{aligned} &\frac{h_0}{\rho\ell\omega} > 1 \\ &J\left(\sqrt{\log\left(\frac{h_0}{\rho\ell\omega}\right)}\right) < \frac{\rho c\sigma\theta_0}{h_0\sqrt{\pi}} < J\left(\sqrt{\log\left(\frac{h_0}{\rho\ell\sigma}\right)}\right) \end{aligned} \tag{21}$$

then the coefficients ε, γ and k are determined by

$$\gamma = \frac{2\theta_o}{\sqrt{\pi}} \left(\frac{\omega}{\sigma} - 1\right) \frac{\xi \exp(-\xi^2)}{\operatorname{erf}(\xi)}$$

$$\varepsilon = \frac{\frac{h_o}{\rho \ell \sigma} \exp(-\xi^2) - 1}{\frac{\omega}{\sigma} - 1} , \quad k = \frac{\rho c \sigma^2}{\xi^2} \tag{22}$$

where $\xi > 0$ is the unique solution of the equation (18), and $\omega > \sigma > 0$ characterize the moving boundaries $r(t) = 2\omega\sqrt{t}$ and $s(t) = 2\sigma\sqrt{t}$ respectively.

2.6 Determination of unknown thermal coefficients through approximate methods in a one-phase Lame-Clapeyron problem

We want to determine formulas for the unknown thermal coefficients through the following approximate methods: Stefan's quasi-stationary method (Q-SM) [66, 67], Goodman's balance integral method (BIM) [36, 37] and Biot's variational method (VM) [4,5,56].

Problem P7 This is the same problem P3 or P4 but now considering the Q-SM, BIM and VM.

REMARK 4 The results corresponding to problem P7 are given in [33]. Moreover, a comparison of these results with the explicit solutions is also given with an analysis of the range of temperatures stated in [32].

In conclusion, we can say that Section 2 of this paper can be considered to represent an interaction between mathematics and engineering.

NOMENCLATURE

$a^2 = \frac{k}{\rho c}$: thermal diffusivity

c : specific heat

k : thermal conductivity

ℓ : latent heat of fusion

q : heat flux

s : position of phase-change location

t : time

x : spatial variable

ρ : mass density

θ : temperature

Subscripts

i=1 : solid phase

i=2 : liquid phase

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