Gasdynamic perturbations in laser-induced vaporization processes

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Vaporisation of condensed substances heated by laser or electron beams is widely used for various practical purposes. Theoretical description of these processes is complicated, in particular, due to non-equilibrium nature of intense evaporation which manifests itself in metastable states of condense and vapour phases as well as in Knudsen layer (KL) jump adjacent to evaporating surface. In the framework of fluid dynamics KL is considered as discontinuity where appropriate boundary conditions should be formulated to describe phase transition kinetics which depends on gas flow dynamics.

For sonic and supersonic vapour flow with Mach number $M \geq 1$ gas-dynamic effects are irrelevant to the condensed phase behaviour. A linear response of such vaporisation process to small modulation of the radiation intensity was considered in Ref. 1 in the framework of one-dimensional heat conduction approach and it was shown that the surface pressure and temperature response has a resonant behaviour with respect to the modulation frequency. Resonances in laser penetration were observed later in different experiments[2-4]. Many effects can contribute to such behaviour: plasma screening melt expulsion, and others[2-4]. In this paper it is shown that one-dimensional gas-dynamic effects at $M<1$ also enhance resonant-like response of the vaporisation process described earlier in Ref.1 for the case $M=1$.

Boundary conditions at the vaporisation front can be obtained from conservation laws for mass g_1, momentum g_2 and energy g_3 fluxes if nonequilibrium distribution function f_{ne} is known at the inner side of KL. In phenomenological approaches f_{ne} is approximated by various model expressions[5-7]. Many papers (see e.g. Ref. 5-11 and references therein) are devoted to theoretical and experimental investigations of KL.

In Ref. 5 f_{ne} has a form of shifted Maxwellian $f(n^*, u^*, T_z, T_{xy})$ with mean concentration n^*, mean velocity u^* along z axis and two different temperatures T_z and T_{yz} for motion in z direction and xy plane. These four parameters are subjected to three conditions: mass $g_1^{(+)}$, momentum $g_2^{(+)}$ and energy $g_3^{(+)}$ fluxes evaluated with the help of f_{ne} in positive $v_z \geq 0$ velocity half-space should be the same as obtained with the help of equilibrium (saturated) half-Maxwellian $f_0^{(+)}=f_0(n_s, T_s)$, $v_z \geq 0$, where n_s is saturated vapour concentration at the surface with temperature T_s.

Another approach is used in Ref. 6 where positive $f_{ne}^{(+)}$ part ($v_z \geq 0$) of f_{ne} is equal to $f_0^{(+)}(n_s, T_s)$, while $f_{ne}^{(-)}$ for particles moving to surface $z=0$ is proportional to equilibrium shifted Maxwellian $f(n,u,T)$ at the outer side of KL, $f_{ne}^{(-)}=\beta f(n, u, T)$, $v_z \leq 0$. Parameter $\beta(M)$ changes from 1 to 6.28 as M grows from 0 to 1. In this model g_1, g_2, and g_3 have extrema at $M=0.88$, 1.18, and 1.22 respectively, while in Ref. 5 all g_i have extrema at the same point $M=1$.

This difference between Ref. 5 and Ref. 6 was pointed out in Ref. 7 where it was shown that a simple model with $f_{ne}^{(+)}=f_0^{(+)}(n_s, T_s)$ and $f_{ne}^{(-)}=\alpha^7 f_0(n_s, \alpha^2 T_s)$, $v_z \leq 0$ also gives extrema for all $g_i(M)$ at $M=1$. The models [5,7] with g_i extrema at $M=1$ seem to be more preferable than model[6].

Vaporisation boundary conditions determine $g_i(T_s, M)$ as functions of T_s and M. At phase equilibrium $M=g_1=g_3=0$ and g_2 is saturated vapour pressure $p_s(T_s)$. In the case of time-dependent surface temperature $T_s=T_0+\delta T_s e^{i\omega t}$, $\delta T_s < T_0$, Mach number $M(t)=M+\delta M e^{i\omega t}$ is also modulated by the term δM which can be found from linearized gas-dynamic equations for one-dimensional ideal adiabatic flow[12] above the evaporating surface $z=0$:

$$i\omega\delta\rho + u\frac{\partial\delta\rho}{\partial z} + \rho\frac{\partial\delta u}{\partial z} = 0,$$

$$i\omega\delta u + u\frac{\partial\delta u}{\partial z} + \frac{1}{\rho}\frac{\partial\delta p}{\partial z} = 0,$$

(1)

$$(i\omega + u\frac{\partial}{\partial z})(\delta p - u_c^2\delta\rho) = 0.$$

For perturbations of gas pressure δp, velocity δu, and density $\delta\rho$ this procedure gives:

$$\frac{\delta p}{p} = A_1 e^{-ik_1 z} + A_2 e^{-ik_2 z}, \quad \frac{\delta u}{u} = \frac{1}{\gamma M}\left(A_1 e^{-ik_1 z} - A_2 e^{-ik_2 z}\right),$$

(2)

$$\frac{\delta\rho}{\rho} = \frac{\delta p}{\rho u_c^2} + A_3 e^{-ik_3 z}, \quad k_{1,2} = \frac{\omega}{u \pm u_c}, \quad k_3 = \frac{\omega}{u}$$

where $z>0$ is the distance from the surface (or the outer side of KL) and modulation δV of the vaporisation front velocity V is neglected.

For subsonic flow $M<1$ one should put $A_2=0$ because there are no perturbations going to $z=0$ surface from infinity. Using linearized form of the vaporisation boundary conditions for $p(T_s,M)$ and $u(T_s,M)=Mu_c$, $u_c^2=\gamma p/\rho$, one obtains:

$$A_1 = \left(\tilde{p}_s' + \frac{\gamma M}{2}\right)\frac{\delta T_s}{2T_s} + \left(\tilde{p}' + \gamma M + \frac{\gamma M}{2}\tilde{T}'\right)\frac{\delta M}{2M},$$

$$A_3 = \left(\frac{\gamma-1}{\gamma}\tilde{p}_s' - 1\right)\frac{\delta T_s}{T_s} + \left(\frac{\gamma-1}{\gamma}\tilde{p}' - \tilde{T}'\right)\frac{\delta M}{M},$$

(3)

$$\frac{\delta M}{M} = \alpha\frac{\delta T_s}{T_s}, \quad \alpha = \frac{\tilde{p}_s' - \gamma M/2}{\gamma M(\tilde{T}'/2 + 1) - \tilde{p}'},$$

$$\tilde{p}_s' = \frac{\partial\ln p_s}{\partial\ln T_s}, \quad \tilde{p}' = \frac{\partial\ln p}{\partial\ln M}, \quad \tilde{T}' = \frac{\partial\ln T}{\partial\ln M}$$

If $g_i(T_s, M)$ have extrema at $M=1$ as it is the case for the models[5,7] then A_1 and A_3 become independent of $\delta M\neq0$ at this point where $\tilde{p}' = -5/4$ and $\tilde{T}' = -1/2$. From (3) it is also seen that the gas-dynamic perturbations enhance vaporisation process because $\alpha>0$.

Consider now time-dependent vaporisation process induced by surface heating with modulated intensity $I(t)=I+\delta I e^{i\omega t}$, $\delta I<I$. Temperature distribution in evaporated condensed matter is determined by one-dimensional Stefan-like problem

$$\frac{\partial T}{\partial t} + V\frac{\partial T}{\partial z} = \chi\frac{\partial^2 T}{\partial z^2}, \quad c\rho_0\chi\frac{\partial T}{\partial z}\bigg|_0 + \rho_0 LV = I, \quad T(t,-\infty) = T_\infty,$$

(4)

where thermal diffusivity χ, specific heat c, and density ρ_0 are supposed to be constant while latent heat $L(T_s,M)$ as well as vaporisation front velocity $V=g_1/\rho_0$ depend on T_s and M. At $M=1$ front velocity $V(T_s)=V_B\exp[A(1-T_B/T_s)]$, where T_B is normal boiling temperature, $A\sim3L/cT_B\sim10$ and $V_B\sim(0.8p_s/\rho_0 u_c)\cdot(\gamma/2\pi)^{1/2}\sim1$cm/s for metals, e.g. for Pb.

Despite this extra dependence of L and V on M the problem (4) after linearization can be reduced to that considered in Ref. 1 because $\delta M=\alpha M\delta T_s/T_s$[13]. Taking into account this relation one obtains for δT_s the same expression as in Ref. 1:

$$\delta T_s = \frac{\delta T}{g}\phi, \quad \phi^{-1} = 1 + (n-1)\left(a - \frac{b}{1+n}\right), \quad n^2 = 1 + \frac{4i\omega\chi}{V^2},$$

(5)

$$b = 2aT_s\frac{V'}{V} = \rho_0 c\Delta T\frac{V'}{g}, \quad g = [(L+c\Delta T)\rho_0 V]', \quad \Delta T = T_s - T_\infty$$

where prime in expressions for b and g now means total differentiation with respect to T_s:

$$V'(T_s, M) \equiv \frac{\partial V}{\partial T_s} + \alpha \frac{M}{T_s} \frac{\partial V}{\partial M} \tag{6}$$

At given value of T_s this modification changes coefficients $a<b<1$ and increases maximum value ϕ_m of the response function modules $|\phi(\omega_m)|$ which can be expressed approximately by the formula

$$\phi_m \cong [1 - b(1-r)^2]^{-1}, \quad r^2 = a/b. \tag{7}$$

The increase of ϕ_m is more pronounced at $M \ll 1$ and it is connected with the fact that the total derivative V' is greater than the partial derivative with respect to T_s. This difference tends to zero as M approaches unity if g_i have extrema at this point while at $M \ll 1$ value of $\phi_m -1$ is approximately as twice as much as at $M=1$.

Maximum ϕ_m and resonance frequency ω_m as functions of M are shown on Figs. 1 and 2 respectively for above mentioned boundary conditions[7] with the specific-heat ratio $\gamma=5/3$ and for the same material constants as in Ref. 1.

It is worthwhile to mention in conclusions that such an enhancement of the vaporisation response due to gas-dynamic reaction is in contrast to the Le Chatellier principle for equilibrium systems: the surface temperature modulation δT_s gives rise to the Mach number change δM which increases the effect of δT_s on vaporisation process. Such a behaviour is pertinent to unstable systems or processes. In fact, at $M<1$ vapour flow becomes unstable for the same reason which makes unstable planar flame front in slow combustion regime (Darreius-Landau instability). The stability problem of the vaporisation front at $M<1$ will be considered below.

In the considered problem liquid phase behaviour is described by the heat conduction and Euler equation with constant density ρ_l, thermal diffusivity χ, and specific heat c and vaporisation boundary conditions. In the case of stationary plane evaporating front its temperature is determined from Eq. (4) $T_l = \Delta T[\exp(k_0 z) - 1] + T_s$, where

$\Delta T = T_S - T_\infty$ is the difference between the surface temperature T_S and $T_\infty = T(z = -\infty)$, $k_0 = V/\chi$.

If the surface parameters perturbations are proportional to $\exp(\omega t - ikx)$. Thin linearized boundary conditions can be written as

$$\delta v_z = \omega \xi + \delta g_1 / \rho_1,$$

$$\delta p_1 = \delta g_2 - 2\nu \delta g_1 + \sigma k^2 \xi, \quad z = 0 \tag{8}$$

$$\delta(g_1 L_{ne}) + c\rho_1 \chi \left(\frac{\partial \delta T_1}{\partial z} + \frac{\partial^2 T_1}{\partial z^2} \right) = 0$$

where non-equilibrium latent heat

$$L_{ne} = L(T_S) + c(T - T_S) + (u^2 - v^2)/2 = L(T_S) + g_3 / g_1 - cT_S - v^2 / 2$$

(the last term will be neglected later on) and ξ is the surface displacement with respect to the unperturbed front $z=0$, so that $\delta T_S = \delta T_1(0) + \xi \, \delta T_1 / \delta z$. From (8) it follows

$$\delta v_z = \delta v e^{kz}, \quad \delta v_x = -i\delta v e^{kz}, \quad \delta p_1 = -\frac{\rho_1}{k}(\omega + kv)\delta v e^{kz},$$

$$\delta T_1 = \frac{k_0 \Delta T \delta v}{\omega - kv} \left(e^{qz} - e^{(k+k_0)z} \right) + (\delta T_S - \xi k_0 \Delta T) e^{qz} \tag{9}$$

where q is determined from the equation $q^2 - qk_0 - k^2 - \omega/\chi = 0$ with Re $q>0$.

Eqs.(8),(9) are not closed because δg_1, δg_2 and δL_{ne} depend on Mach number perturbation δM which can be found from closed set of equations for liquid and vapor phases. Vapor flow is described by gasdynamic equations for an ideal gas with $\gamma = c_p/c_v = \rho u_c^2 = 5/3$ where u_c is the sound velocity. In the unperturbed vapor flow mass density ρ, pressure p, velocity component $u_z = u = g_1/\rho$ and Mach number $M = u/u_c$ are constant.

For linearized boundary conditions and gas flow perturbations one has

$$\delta p = \delta(g_2 - g_1 u), \quad \delta u_z = \omega\xi + \delta u, \quad \delta u_x = \delta v_x + ik(u-v)\xi,$$

$$\delta p = \sum_{i=1,2} A_i e^{-k_i z}, \quad \delta\rho = \frac{\delta p}{c_g^2} + A_3 e^{-k_3 z}, \tag{10}$$

$$\delta u_z = \sum_{i=1,2} A_i \frac{k_i}{\rho(\omega - k_i u)} e^{-k_i z} + \frac{ku}{\omega} A_4 e^{-k_3 z}, \quad z \geq 0$$

$$\delta u_x = \sum_{i=1,2} A_i \frac{ik}{\rho(\omega - k_i u)} e^{-k_i z} + iA_4 e^{-k_3 z}, \tag{11}$$

where k_3 and k_i, $i=1,2$ are given by the relations

$$k_3 = \frac{\omega}{u}, \quad (u_c^2 - u^2)k_i^2 + 2k_i\omega u - \omega^2 - k^2 u_c^2 = 0 \tag{12}$$

In Eq. (11) $A_2=0$ for the same reason as in Eq. (2) $A_2=0$. From Eqs. (8-12) it follows a homogeneous set of equations for δv, ξ, δT_S, δM:

$$\delta v - \omega\xi = \delta g_1 / \rho_1,$$

$$\delta v\rho_1(v + \omega/k) + \sigma k^2\xi = -\delta g_2 + 2v\delta g_1$$

$$\delta(g_1 L_{ne}) + c\rho_1\chi\left(\frac{k_0\Delta T\delta v}{\omega - kv}(q - k - k_0) + q\delta T_S + \xi k_0\Delta T(k_0 - q)\right) = 0 \tag{13}$$

$$\delta u_x = \frac{i\omega}{ku}(\omega\xi + \delta u) - \frac{i\delta(g_2 - g_1 u)}{\rho u}F = -i\delta v + ik(u-v)\xi,$$

where

$$\delta \ln g_1 = (\bar{p}_S' - 0.5)\delta \ln T_S + \bar{g}_1'\delta \ln M, \quad \bar{g}_1' = 1 + \bar{p}' - 0.5\bar{T}',$$

$$\delta \ln g_2 = \bar{p}_S'\delta \ln T_S + \bar{g}_2'\delta \ln M, \quad \delta \ln L_{ne} = \bar{L}\delta \ln T_S + \bar{L}\delta \ln M,$$

$$\bar{g}_2' = \left(\bar{p}' + \frac{2\gamma M^2}{\gamma M^2}\right), \quad \bar{L}' = \frac{c_p T}{L_{ne}}\left(\bar{T}' + \frac{2M^2}{3}\left(1 + \frac{\bar{T}'}{2}\right)\right), \tag{14}$$

$$\delta \ln u = 0.5\delta \ln T_S + (1 + 0.5\bar{T}')\delta \ln M, \quad F = \frac{k_1\omega - k^2 u}{k(\omega - k_1 u)},$$

and the notations $\bar{H}_S'$, $\bar{H}'$ mean respectively $\bar{H}_S' = \partial \ln H / \partial \ln T_S$, $\bar{H}' = \partial \ln H / \partial \ln M$ for any function $H(T_S, M)$.

The set (13) has a nontrivial solution if its determinant is zero. This condition gives rise to a characteristic equation which determines the dispersion function $\omega(k)$. At $\Delta T=0$ and $V \ll u$ the function $\omega(k)$ is determined by the relation

$$f(\omega, k) + \frac{\delta \ln M}{\xi}\frac{\delta \ln T_S}{\delta \ln M}\left[(\bar{p}_S' - 0.5)u(\omega + kv) + \frac{k}{\rho_1}g_2\bar{p}_S'\right] +$$

$$\frac{\delta \ln M}{\xi}\left[\frac{k}{\rho_1}g_2\bar{g}_2' + \bar{g}_1'u(\omega + kv)\right] = 0, \tag{15}$$

where

$$f(\omega, k) = \omega^2 + \omega kv + \sigma k^3 / \rho_1,$$

$$\frac{\delta \ln T_S}{\delta \ln M} = -\frac{g_1(L_{ne}\bar{g}_1' + \bar{L}')}{qT_S c\rho_1\chi + g_1(L_{ne} - L(T_S) + (\bar{p}_S' - 0.5)L_{ne})}, \tag{16}$$

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and $\delta\ln M/\xi$ is given by the relation

$$\frac{\omega^2}{ku} + \omega - ku + \frac{\delta\ln M}{\xi}\frac{\delta\ln T_S}{\delta\ln M}\left[-p\frac{\overline{p}_S{}'}{g_1}F + u(\overline{p}_S{}' - \frac{1}{2}) + \frac{\omega}{2k}\right] +$$

$$\frac{\delta\ln M}{\xi}\left[-p\frac{\overline{p}{}'}{g_1}F + \frac{\omega}{k}\left(1 + \frac{\overline{T}{}'}{2}\right) + u\overline{g}_1{}'\right] = 0.$$

(17)

At small Mach number M≪1 from (15), (16) it follows $\omega^2 + 2\omega kV + \sigma k^3/\rho_1 - k^2 uV = 0$. This formula coincides with Darreirs-Landau equation. Taking into account the extremal properties of g_1 at M=1 one obtains from (15),(16) the relation $f(\omega,k)=0^{14}$.

Gasdynamic effect on liquid surface behaviour in eqs (15),(16) becomes negligible at M=1 also in the case $\Delta T\neq 0$, i.e. the problem (8),(9) becomes closed because $g_1(M=1)=0$. It should be noted that $\delta M\neq 0$ at M=1. This result was not obtained in Ref. 15 because of inadequate treatment of boundary conditions. A detailed analysis of the obtained dispersion equation will be presented elsewhere.

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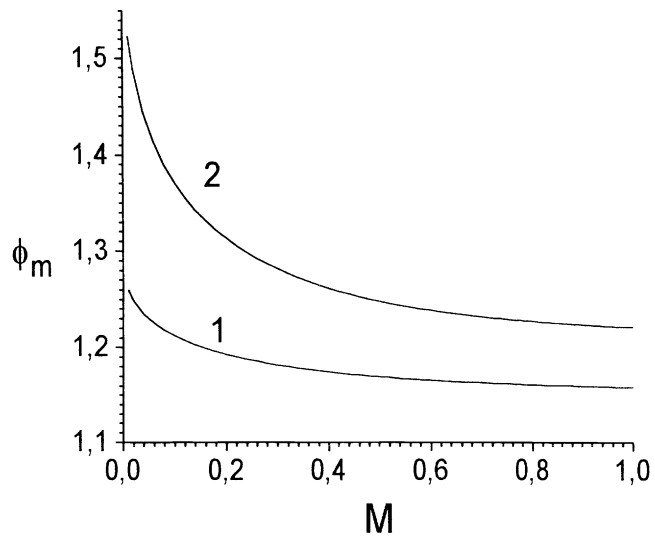
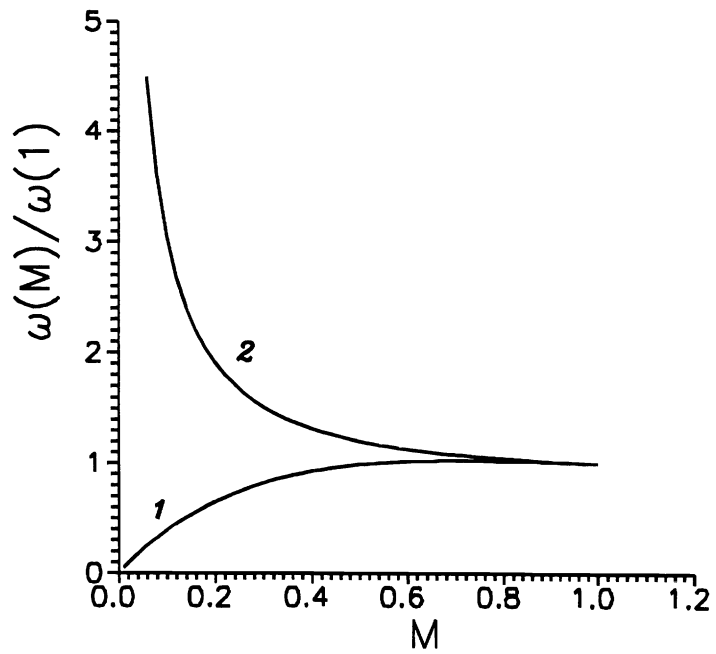Fig.1: Dependence of ϕ_m on M at $T_S/T_B=1$ (plot 1) and 2 (plot 2).

Fig.2: Dependence of normalized resonance frequency $\omega(M)/\omega(1)$ on M at $T_S=T_B$ (plot 1) and I=const (plot 2) with $T_S=T_B$ at M=1