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Droplet evolution in a liquid/vapor aluminum flow

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Abstract

We have made estimates of surface effects and droplet evolution in the two-phase flow that should be observed in the upcoming foil heating experiments planned for the NDCXII machine at LBNL. An aluminum foil of order micron thickness will be heated by a heavy ion beam to the 1 eV range. The expansion will take place in the two-phase regime (gas/liquid), so the heated metal will first melt, then fragment into droplets, and then the droplets will undergo some evaporation. We propose hydrodynamic criteria to estimate the maximum size of the droplets (~100 nm), considering a balance between hydrodynamic disruptive forces and restoring surface tension. We estimate the relevant thermodynamic functions (surface tension, latent heat, viscosity) for temperatures up to the critical temperature, and we use them to make a simple model for the partial or total evaporation of a droplet in the expanding flow.
Outline

1. Introduction: Warm Dense Matter (WDM) studies

2. Expected qualitative hydrodynamics of metals expanding in a two-phase flow. Maximum size of droplets.

3. Estimates of needed physical quantities:
   - $\sigma$ - surface tension
   - $L$ - latent heat
   - $\mu$ - viscosity

   1. Low temperature case ($< T_c$ = critical temperature)
   2. High temperature case ($> T_c$)
NDCX II is a planned accelerator designed to reach uniform warm dense matter conditions.

<table>
<thead>
<tr>
<th>Ion Beam</th>
<th>A</th>
<th>Energy at Bragg Peak</th>
<th>dE/dX at Bragg Peak</th>
<th>Foil Entrance Energy (approx)</th>
<th>(\Delta z ) for 5% variation (10% solid Al)</th>
<th>Beam Energy for T=10 eV/mm(^2)</th>
<th>(t_{\text{hydro}}) at 10 eV</th>
<th>Beam Power per mm(^2)</th>
<th>Beam Current for 1 mm diameter spot</th>
<th>Line Charge Density at Focus</th>
<th>Density at Focus</th>
</tr>
</thead>
<tbody>
<tr>
<td>Li</td>
<td>6.94</td>
<td>1.9</td>
<td>2.05</td>
<td>2.9</td>
<td>34.3</td>
<td>5.7</td>
<td>0.8</td>
<td>6.8</td>
<td>1860.7</td>
<td>2.09E-04</td>
<td>1.66E+15</td>
</tr>
<tr>
<td>Na</td>
<td>22.99</td>
<td>15.9</td>
<td>11</td>
<td>23.9</td>
<td>53.5</td>
<td>8.9</td>
<td>1.3</td>
<td>6.8</td>
<td>222.3</td>
<td>1.57E-05</td>
<td>1.25E+14</td>
</tr>
<tr>
<td>K</td>
<td>39.10</td>
<td>45.6</td>
<td>18.6</td>
<td>68.4</td>
<td>90.8</td>
<td>15.1</td>
<td>2.2</td>
<td>6.8</td>
<td>77.5</td>
<td>4.22E-06</td>
<td>3.35E+13</td>
</tr>
</tbody>
</table>
Strategy: maximize uniformity and the efficient use of beam energy by placing center of foil at Bragg peak.

In simplest example, target is a foil of solid or “foam” metal.

Example: Ne

Energy loss rate

\[ \frac{1}{Z^2} \frac{dE}{dX} \]

(MeV/mg cm²)

\( \Delta dE/dX \propto \Delta T \)

In example,

\( E_{\text{entrance}} = 1.0 \text{ MeV/amu} \)
\( E_{\text{peak}} = 0.6 \text{ MeV/amu} \)
\( E_{\text{exit}} = 0.4 \text{ MeV/amu} \)

\( (\Delta dE/dX)/(dE/dX) \approx 0.05 \)

(dEdX figure from [2])
Two-phase WDM target hydrodynamics

\( \rho \) and \( T \) evolution of a plane WDM target (DPC simulation result) (cf. [3])

Reference case:
- **beam**: Li+ at 2.8 Mev/ion
- **target**: 3.5 \( \mu \)m-thick aluminum foil
- **pulse length**: 1 ns
- **focal spot**: \(~1\) mm
Discontinuity in temperature decay power law has motivated investigation of 2-phase behavior

- Fast decay (I: approx -2/3) and then slow decay (II: approx -1/3)
- Change in slope (kink) corresponds to moment when center of the foil enters the 2-phase region

From liquid to 2-phase regime (reference case):
- Position of kink: on the border

<table>
<thead>
<tr>
<th>Position</th>
<th>1 ns</th>
<th>0.8 ns</th>
<th>0.6 ns</th>
<th>0.4 ns</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 ns</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.2 ns</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
How can we describe the 2-phase hydrodynamics?

- The foil will melt then enter 2-phase conditions.
- First, bubble form (B), then the continuous liquid fragments into droplets (D)
Bubbles or droplets?

Separation line is where each phase occupies half of the volume

First bubbles form, but then quickly droplets form everywhere, (always for \( \rho \ll 1 \text{ g/cm}^3 \), for these parameters)
Maximum size of a droplet in a diverging flow?

- Equilibrium between stretching viscous force and restoring surface tension:
  - Capillary number $\text{Ca} = \text{viscous/surface} \sim \int \mu \frac{dv}{dx} x \, dx / (\sigma x) \sim (\mu \frac{dv}{dx} x^2)/(\sigma x) \sim 1$
  - Maximum size:
    \[
    x = \sigma / (\mu \frac{dv}{dx})
    \]
    (cf. [4], [5])
    → Estimate: $x_{\text{max}} \sim 0.2 \, \mu m$

AND/OR:

- Equilibrium between disruptive dynamic pressure and restoring surface tension: Weber number $\text{We} = \text{inertial/surface} \sim (\rho v^2 A) / \sigma x \sim \rho (\frac{dv}{dx})^2 x^4 / \sigma x \sim 1$
  - Maximum size:
    \[
    x = (\sigma / \rho (\frac{dv}{dx})^2)^{1/3}
    \]
    (cf. [6])
    → Estimate: $x_{\text{max}} \sim 0.05 \, \mu m$
Typical conditions for droplet formation:
t=1.6 ns, T=1 eV, ρ_{liq} = 1 g/cm^3

- Surface tension: σ ≈ 100 dyn/cm
- Thermal speed: v ≈ 5 \times 10^5 cm/s
- Viscosity: Kinetic gas: m = \frac{1}{3} m v^* n l 
  mean free path : l = \frac{1}{\sqrt{2}} n \sigma_0 
  \rightarrow \mu = \frac{m v}{(3 \sqrt{2} \sigma_0)} = 27 \times 1.67 \times 10^{-24} \times 5 \times 10^5 / (3\sqrt{2} \times 10^{-16}) 
  \mu \approx 5 \times 10^{-3} g/(cm-s)
- Velocity gradient: \frac{dv}{dx} = 10^6 \text{ cm/s} / 10^{-3} \text{ cm} 
  \frac{dv}{dx} = 10^9 \text{ s}^{-1}

→ Conclusion: Maximum size is expected to be \approx 0.1 \mu m
Liquid and vapor density boundary in Al

Taken from the EOS used in the DPC code: obtained by maxwellian construction
Surface tension of liquid aluminum

Curve obtained by fitting universal law for simple liquids (principle of corresponding states) with data at low temperature and value of critical temperature $T_c$ (cf. [7])

$$\sigma = \sigma_0 (1 - T/T_c)^{1+r} \quad \text{with} \quad r = 0.27$$

From CRC Handbook in chemistry and physics (1964)
Latent heat is nearly linear

Latent heat of vaporization of liquid Aluminum

Assumption: L and \( \sigma \) are both proportional to the binding energy per particle

\[
L \propto \sigma \times n^{-2/3}
\]

\([J/\text{particle}] \quad [J/m^2] \quad \text{[particles/m}^3\text{]}^{-2/3} \]

Slope obtained: \(-4.33\) J/K/atom \(\approx 3\ k_B\): consistent with model

Curve obtained by multiplying \( \sigma(T) \) (see previous slide) by \( \rho^{-2/3} \) (taken from EOS in DPC) and adjusting with experimental value at low temperature
Viscosity of liquid and vaporized Aluminum

Experimental values for liquid

Viscosity in the Warm Dense Matter ranges (liquid and gas) is difficult to evaluate!
Model equations for evaporation and condensation of droplets (preliminary equations)

\[ V(t) = \text{volume of gas} + \text{volume of liquid drop} \]

\[ \rho_g(T) = mn_g(T) \text{ and } \rho_l(T_l) = mn_l(T_l) \text{ taken from 2-phase boundary in EOS} \]

**Kelvin's equation:**

\[ \ln\left( \frac{P_{\text{curved}}}{P_{\text{flat}}} \right) = 2\frac{\sigma}{n_l k T_l} \]

\[ \rightarrow n_{gsat} = n_g(T_l)e^{[2\sigma/(n_l k T_l R_l)]} \]

Contains all the physics of surface effects for the droplets!

 Flux of particles onto droplet:

\[ \Phi_{\text{cond}}(m_g, T_g) = m_g/(mV_g) \left( k_B T_g / 2\pi m \right)^{1/2} \]

Flux of particles evaporating off of droplet:

\[ \Phi_{\text{vap}}(T_l) = n_{gsat}(T_l) \left( k_B T_l / 2\pi m \right)^{1/2} \]

Volume of liquid:

\[ V_l(m_l, T_l) = 4\pi R_l^3 / 3 = m_l/(mn_l(T_l)) \]

Surface area:

\[ S_l = 4\pi R_l^2; \quad V_g(m_l, T_l, t) = V(t) - V_1(m_l, T_l) \]
Model equations

1) \[ \frac{d}{dt}(m_l + m_g) = 0 \]  
   mass conservation

2) \[ \frac{dm_l}{dt} = m \beta (-\phi_{vap} + \phi_{cond}) S_l \]  
   vaporization condensation

3) \[ \frac{d}{dt}\left(\frac{m_l}{m} c_{vl} T_l\right) = \beta \left(-\left(L_0 + c_{vg} T_l\right) \phi_{vap} + \left(L_0 + c_{vg} T_g\right) \phi_{cond}\right) + (1 - \beta) \alpha \phi_{cond} c_{vg} (T_g - T_l) \]  
   vaporization condensation thermalization by non-sticking particles

4) \[ \frac{d}{dt}\left(\frac{m_g}{m} c_{vg} T_g\right) = \beta \left(c_{vg} T_l \phi_{vap} - c_{vg} T_g \phi_{cond}\right) - (1 - \beta) \alpha \phi_{cond} c_{vg} (T_g - T_l) \]  
   vaporization condensation thermalization by non-sticking particles

\[ + \frac{\partial E}{\partial V_g} \frac{\partial V_g}{\partial t} + \frac{\partial E}{\partial V_g} \frac{\partial V_g}{\partial m_g} \frac{\partial m_g}{\partial t} \]

prescribed adiabatic expansion compression heating by vaporizing gas

\[ m_l, \ T_l = \text{mass, temperature of liquid drop}; \]
\[ m_g, \ T_g = \text{mass, temperature of gas}; \]
\[ m = \text{atomic mass of material}; \]
\[ \alpha = \text{thermalization coefficient}; \]
\[ \beta = \text{sticking coefficient}; \]
\[ c_{vg} = \text{heat capacity of the gas} = 3/2 \ k_B \]
\[ c_{vl} = \text{heat capacity of the liquid} = 3 \ k_B \]
Why do escaping particles take away $L_0 + c_{vg}T_l$ from liquid?

Mean energy of particles that escape from potential well of depth $L_0$ will have mean energy $\sim kT_l$ relative to gas zero point.

$L_0 = \text{latent heat of liquid particles}$

0 point of KE for particles within liquid

0 point of KE for particles within gas

Mean atomic separation

Energy

$kT_l$

$n(E)$

Maxwell-Boltzmann distribution

(1 to 1.5)$kT_l$
1. Low initial temperature \( (T<T_c) \): results of the Mathematica model for the evaporation of a droplet

Assumptions: \( \alpha=0.5, \beta=0.5; \) at \( t=0 \): \( V_{g0}=V_{l0}=4\pi X_0^3/3; \) \( X_0=0.1 \mu m; \) \( T_{g0}=T_{l0}=10000K \)

It says... droplets do not evaporate completely → Persisting “bullets” (?)
Model equations show that very small droplets evaporate, whereas larger ones persist.

Assumptions: \( \alpha = 0.5, \beta = 0.5; \)

at \( t=0: \quad V_{g0} = V_{l0} = 4\pi X_0^{3/3}; \quad T_{g0} = T_{l0} = 10000K \)
Importance of the thermalization from liquid to gas

At long times, for droplets
In the reference case, thermalization is efficient: $T_l=T_g$
2. Debris initially at high T and solid density: initially material is vaporized and cools adiabatically

Adiabatic expansion:

\[ P = nkT = P_o \left( \frac{\rho}{\rho_o} \right)^\gamma \Rightarrow \frac{T}{T_0} = \left( \frac{\rho}{\rho_o} \right)^{\gamma^{-1}} \propto \rho^{2/3} \]

Nucleation of droplets?

Standard nucleation theory \( (R_{\text{min}} = 2\sigma/\Delta P) \) is included in the model via Kelvin’s equation
Conclusion

• Criteria for max droplet sizes will need to be compared to observations (this study is only theoretical for the moment)

• Model equations can be used in several different situations: high / low initial temperature, 1-D / 3-D expansion of the cell (3-D when the distance travelled becomes ~ spot radius)

• This study gives tools that should help to understand the upcoming WDM foil heating and other ICF experiments (debris problems)
References

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[7]: F. P. Buff and R. A. Lovett, simple dense fluids (chapter 2: surface tension of simple fluids), 1968