HEIGHTS INTEGRATED MODELS FOR THICK LIQUID WALLS IN IFE SYSTEMS

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Presented at the ARIES Meeting
Princeton, NJ, Oct. 2-4, 2002

HEIGHTS Modeling of Thick Liquid in IFE Systems

1. **Modeling of Liquid Jets Response to Neutron Deposition**

2. **Models of Liquid Jets Fragmentation**

3. **Models Development for Aerosol Formation**

4. **Conclusions & Recommendations**

LIQUID OSCILLATION

● **The following equations of mass, momentum, and energy conservation are solved in HEIGHTS package for the planar, cylindrical, and spherical cases:**

$$
\begin{aligned}
&\frac{d\rho}{dt} + p\,div\vec{V} = 0 \quad , \\
&\rho\frac{d\vec{V}}{dt} + \nabla(p + p_{\mu}) = 0 \quad , \\
&\frac{dE}{dt} + (E + p)\,div\vec{V} = 0 \quad , \\
&p_{\mu} = \frac{B^2}{4\pi}
\end{aligned}
\qquad (1)
$$

where ρ is density, V is velocity, p is pressure, E is the internal energy, and B is external magnetic field if present.

● **The equation of state of 3 components is used assuming that the internal energy consists from thermal motion energy of nuclei, E_i , thermal excitation energy of electrons, E_e, and the elastic energy, E_{cold}. Correspondingly the pressure is also consists of 3 terms, P_i , P_e , and P_{cold} :**

$$
\begin{aligned}
&\mathrm{E} = \mathrm{E_i} + \mathrm{E_e} + \mathrm{E_{cold}}\,(\rho) \\
&E_i = 3nk(T - T_o) + E_o, \;\; E_e = \tfrac{1}{2}\beta_o\left(\frac{\rho_o}{\rho}\right)^{1/2} T^2 \\
&P_i = \Gamma(\rho)E_i \quad , \quad P_e = \tfrac{1}{2}E_e \\
&\Gamma(\mathrm{v}) = -\frac{2}{3} - \frac{\mathrm{v}}{2}\frac{d^2 P_{cold}}{d\mathrm{v}^2} / \frac{dP_{cold}}{d\mathrm{v}} \;,\;\; \mathrm{v} = \tfrac{1}{\rho}, \\
&P_{cold} = P_{xo}\left[\left(\frac{\rho}{\rho_o}\right)^n - 1\right] \;,\;\; P_{xo} = \tfrac{1}{n}\rho_o C_{so}^2
\end{aligned}
\qquad (2)
$$

where T_0 is initial temperature, E_0 is thermal energy at initial temperature, β_0 is coefficient of electron specific heat, Γ is Gruneisen coefficient, power *n* depends on ρ in general, C_{so} is the sound speed at normal conditions, i.e., at $T = T_o$ and $\rho = \rho_o$.

Cavitation of Liquids

● **A tensile relief wave is initiated by spontaneous arising of cavities. Such problem is well investigated by cavitation theory for vapor bubbles arising in overheated liquids.**

The net work associated with the reversible formation of a spherical cavity of radius r is

$$W = 4\pi r^2 \sigma + \tfrac{4}{3}\pi r^3 (P - P_v) \qquad (1)$$

where P is pressure in liquid (negative), P_v is vapor pressure in cavity (positive), σ is the surface tension. The vapor pressure P_v can be neglected and, therefore, the work W has maximum at the critical radius r*

$$r^* = -\frac{2\sigma}{P} \ , \quad W_{max} = \frac{16\pi}{3}\frac{\sigma^3}{P^2} \qquad (2)$$

● **The cavities coming into being with radius less the critical one, r < r* is disappeared while cavities with r > r* grow freely. The equilibrium distribution of cavities with radius R is**

$$n(r) = N\exp\left(-\frac{W}{kT}\right) \qquad (3)$$

where N is number of particles (atoms/molecules) in liquid.

● **The theory of nucleation gives the rate of critical cavities formation:**

$$\frac{dn}{dt} = \frac{NkT}{h}\exp\left(-\frac{\Delta f + W_{max}}{kT}\right) \qquad (4)$$

where Δf is free energy of activation for motion of an individual particle of liquid away from the cavity surface. The fracture pressure can be estimated as:

$$P_\tau = -\sqrt{\frac{16\pi}{3kT}\frac{\sigma^3}{LnA}}\sqrt{\frac{LnA}{LnA+Ln\tau}} \qquad (5)$$

$$A = \frac{NkT}{h}$$

where τ is the time within which at least one cavity can be expected to appear.

● **For Mercury with σ = 474 erg/cm^2**

$$A = \frac{NkT}{h} = 2.55 \cdot 10^{35},$$

$$P_\tau = P_{\tau o}\sqrt{\frac{LnA}{LnA+Ln\tau}},\ P_{\tau o} = 22.3\,katm$$

For Flibe with σ = 375 erg/cm^2

$$A = \frac{NkT}{h} = 2.2 \cdot 10^{33},$$

$$P_\tau = P_{\tau o}\sqrt{\frac{LnA}{LnA+Ln\tau}},\ P_{\tau o} = 8.7\,katm$$

● **Thus, at negative pressure $P < -P_\tau$ liquids can be fractured (break) due to growth of cavities.**

● **The practical rule is that the fracture pressure in technical working conditions is usually 5-10 times less than theoretical limit due to dissolved gases and impurities. For example, for water P_τ(theory) = 1.32 katm, but P_τ(experiment) is less than 350 atm.**

Fragmentation of Liquids

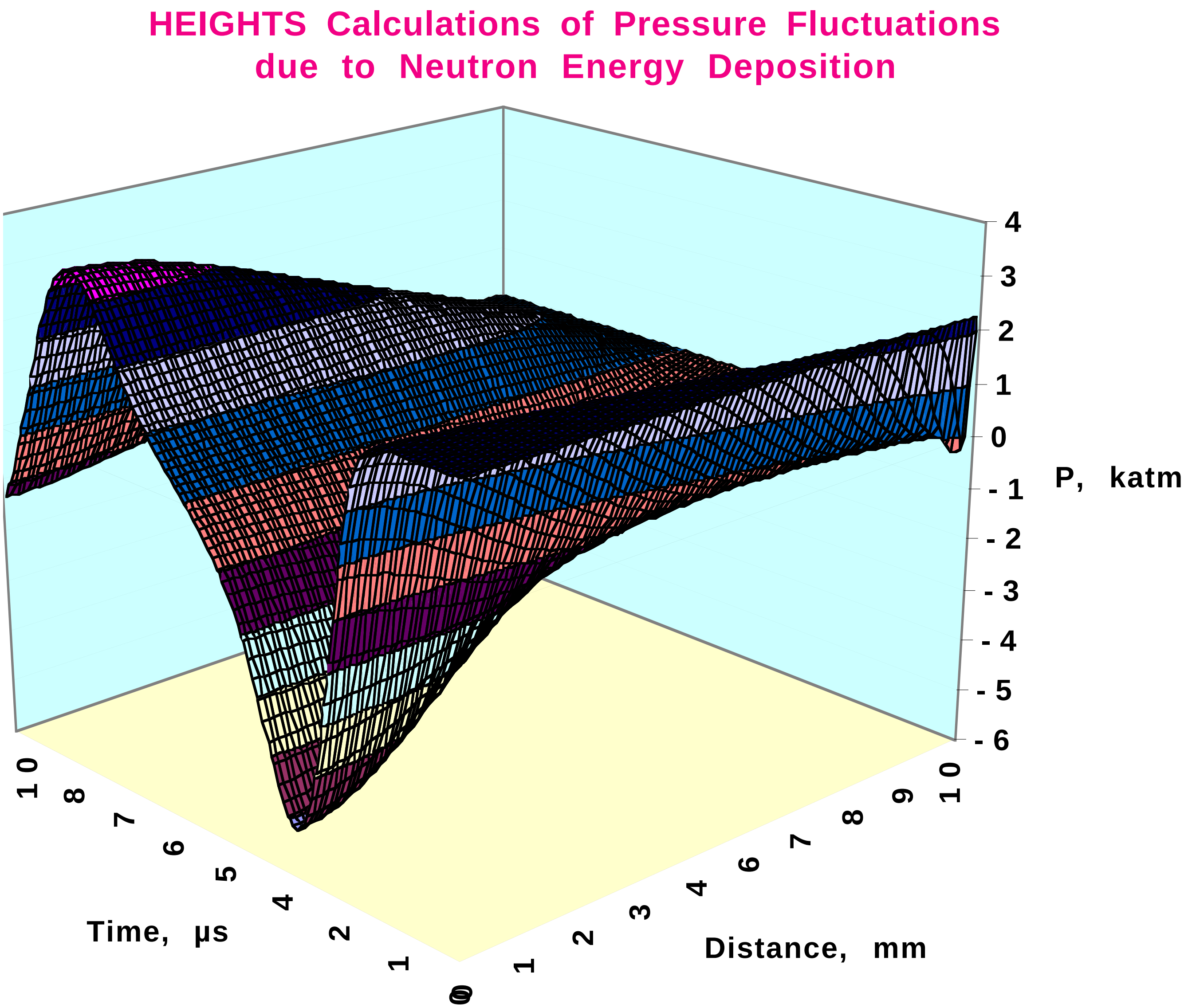
• **Neutron beam volumetric deposition of > 100 J/g in liquid jets resulting thermal pressure rise $P_o \approx$ 2-3 katm that results in negative pressure of –(2-3) P_o at center due to accumulation.**

• **Instant rise of pressure results in excitation of sound waves both in radial, r, and longitudinal, z, directions. During these excitations, pressure oscillates with magnitude $\pm \Delta P_o$ at the surface.**

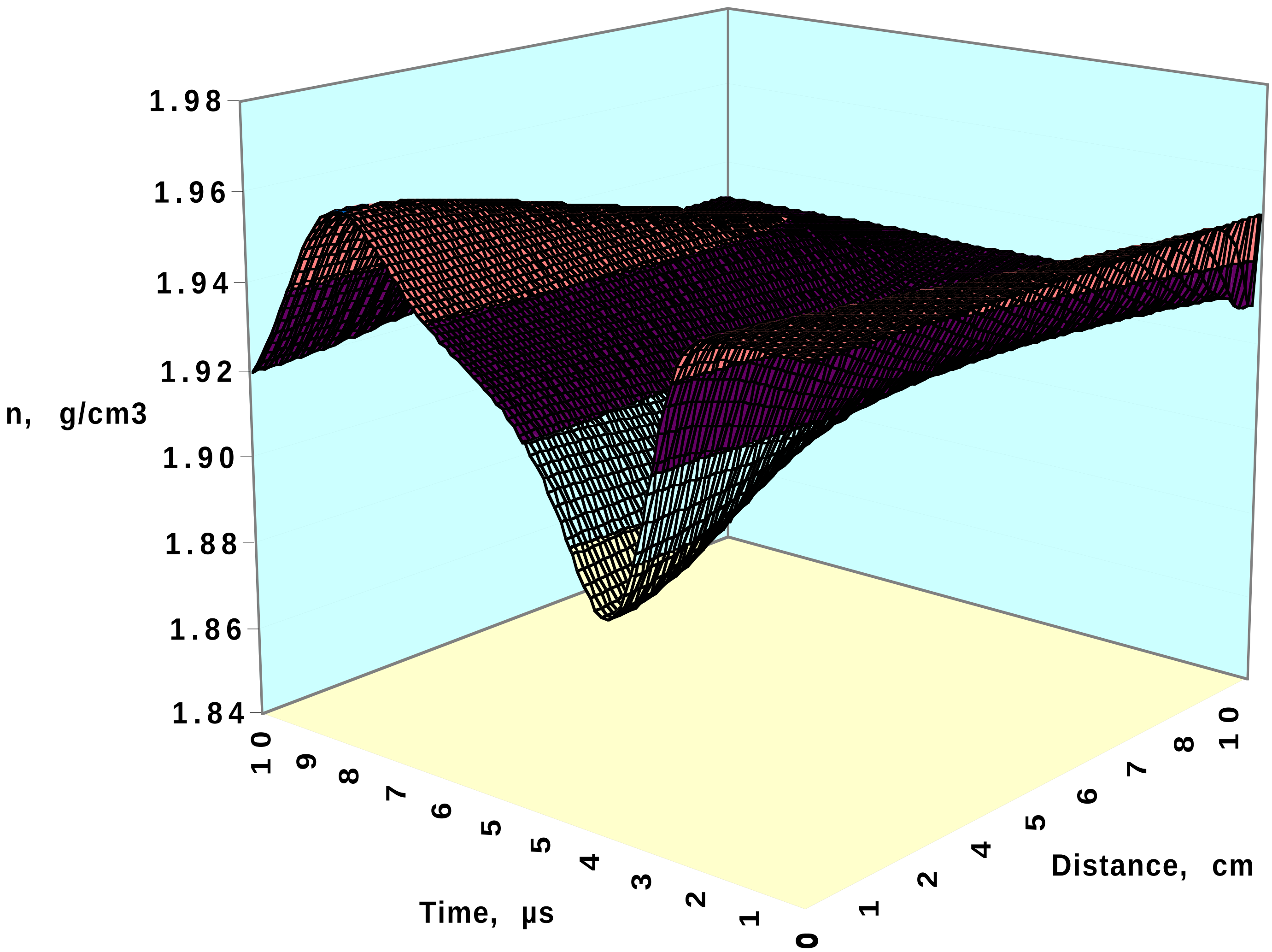
• **Liquid metals subjected to negative pressure are metastable. Spontaneous formation of cavities in stressed liquid can result in fragmentation**

• **Fracture pressure of liquids such as Mercury was measured experimentally by Briggs (P_τ <425 atm) and Carlson (P_τ = 19 katm). Results of Carlson's experiments are in good agreement with Fisher's theory (P_τ = 22.3 katm). Fracture pressure of Flibe is calculated to be P_τ = 8.7 katm.**

• **After neutron deposition and during initial period of few μs, liquid negative tension reaches values near fracture pressure of P_τ.**


HEIGHTS Calculations of Pressure Fluctuations
due to Neutron Energy Deposition
P, katm
4
3
2
1
0
- 1
- 2
- 3
- 4
- 5
- 6
Time, µs
10
8
7
6
5
4
2
1
0
Distance, mm
1
2
3
4
6
7
8
9
10

HEIGHTS Calculations of Flibe Density Fluctuations



Concept of Relaxation Shock Wave

- **A tensile relief wave is initiated by the spontaneously arising of cavities in the stretched media.**

- **Vapor pressure inside cavity can be neglected ($P_{cavity} \approx 0$) and cavity can be considered as empty. However, the liquid outside the cavity is at negative pressure $P_{liquid} = -P$.**

- **Such a jump of pressure results in a *shock wave* with amplitude $P_{shock} = \Delta P$. This shock wave is actually *a relaxation wave* when stretched media at density $\rho < \rho_o$ recovers to normal density, ρ_o.**

- **This relaxation shock wave is driven not by external force as when energy is deposited into target from external sources, but by an internal source of energy equals the elastic strain energy.**

- **Cold pressure returns to zero when density returns to normal value, i.e., the stressed medium returns to normal state by unloading or discharging.**

CAVITY DYNAMICS

- **In usual cavitation theory, vapor bubbles grow with time until they come in region with higher pressure then they collapse which is recognized by measurement of acoustic noise.**

- **Situation under large negative pressure is completely different from cavitation due to vapor bubbles. Vapor bubble grows due to heat conduction from surrounding overheated liquid. Here, empty cavity grows due to unloading of surrounding stretched liquid.**

- **Maximum surface velocity of cavity oscillates with decreasing magnitude as time progresses. The velocity oscillates around a mean value decreasing with time but never becomes negative.**

- **This can be explained as mentioned above that ahead of the cavity the shock wave of relaxation propagates releasing internal energy, i.e., bringing media back to normal state with normal density. *Cavity coming into being never collapse!***

- **The jet as a whole continues to oscillate due to the initial shock but also expands freely releasing its initial energy and converting into kinetic energy of the hollow cavity layer.**

- **Therefore, any arising cavity during the negative pressure stage will not disappear.**

CONSEQUENCIES OF CAVITY EXPANSION

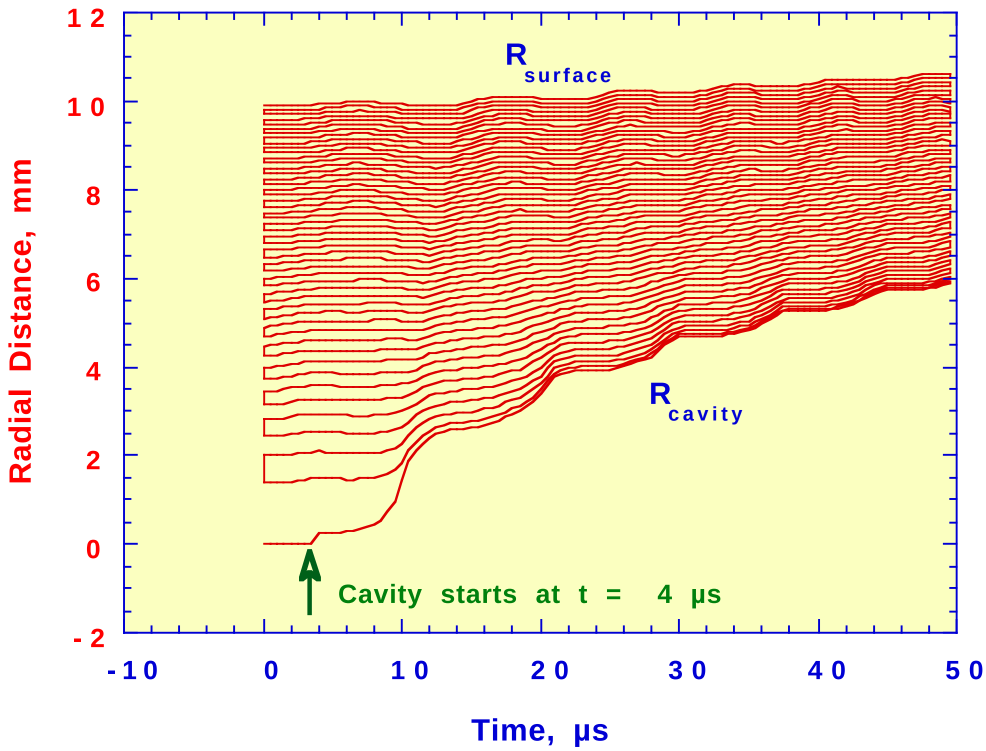
- **Liquid jet will oscillate after instant energy deposition. Because frequency of radial oscillations is much higher than axial oscillations, cavity dynamics is governed mainly by radial oscillations.**

- **During negative pressure phase, a number of cavities can arise spontaneously, mostly near the jet axis where the magnitude of the negative pressure is maximum.**

- **Cavities then expand freely initiating a shock wave of relaxation ahead of cavities surface. Cavities will expand in both radial and axial directions.**

- **At longer time, these cavities can join to form elongated cavity with axial size much more than the radial one. Calculations were made for conditions of Flibe/Flinabe liquid jets.**

HEIGHTS Simulation of Liquid Sphere Dynamics in Presence of a Cavity



Models Development for Aerosol Formation

After X-ray, neutron, and debris energy depositions surface layers are heated to high temperatures exceeding melting, vaporization limits i.e, $T>T_{melt}$, T_{vap}, that results in 4 different mechanisms of fragmentation:

- **During oscillations of liquid layer negative pressure can result in fragmentation due to embryo voids.** (ANL)

- **During non-uniform energy deposition excitation of surface capillary waves can exist resulting in splashing of peaks of nonlinear waves similar to wind splashing of sea surface waves.** (ANL)

- **During vaporization stage, splashing of liquid metal can exist due to volumetric vaporization. Fast vapor bubbles grow in liquid volume until bubble surface reaches the liquid metal surface. Then, vapor bubbles burst and liquid metal jets from bubbles bottom arise. Sausage instability of such jets due to surface tension results in splitting of cylindrical jet into droplets.** (ANL)

- **Vaporized material expands radial toward the chamber center. Cooling of vapor gas during expansion, while gas do not achieves the chamber center, results in vapor condensation below dew point that can form droplets of liquid.** (INEEL)

- **After reaching the center, gas on front of expanding gas-cloud is heated due to stopping. Accumulation near the chamber center makes possible to reach high temperatures. As it follows from calculations of Chen, temperature can reach rather high values of tens eV!** (Berkeley)

- **Resulting shock wave expanding toward the chamber inner surface can result in heating of gas and, consequently, decrease condensation. But** Berkeley **did not take into account ionization and following radiation in detail that decreases temperature and pressure near the center. Dynamics of accumulation with detail radiation are under consideration now to find the real rate of condensation** (NEW-ANL).

FUTURE WORK ON FRAGMENTATION

♦ **Liquid jet fragmentation occurs due to oscillations of liquid after fast energy deposition with duration τ_d less than radial oscillation-time τ_u, i.e.,** $\tau_d < \tau_u = R/C_s$.

♦ Degree of fragmentation is determined by developed negative pressure, pressure limit for fragmentation, and surface tension parameters.

♦ **Up to now an EOS for liquid metals (Flibe/Flinabe) especially under negative pressure is poorly known. Fracture pressure limit depends on liquid purity and surface tension. Such experimental facility is needed to measure and test these parameters.**

♦ **Dynamics of fragmentation can be modeled using multi-dimensional hydrodynamic codes (HEIGHTS) developed that take into account detail features of fragmentation. This includes description of shock and rarefaction waves, viscosity and compressibility limit, dynamics of nucleation, and propagation of relaxation waves.**

♦ **Elaborated models of fragmentation can be verified using existing small or moderate Z-pinch facilities (SNL, LLNL). Another way is to use a wire explosion circuit submerged in Flibe liquid to simulate neutron volumetric energy deposition.**

FUTURE WORK ON AEROSOL

- **Detail integrated study of all possible aerosol formation:**

  - Vaporization
  - Splashing (HD instabilities, bubbles, solid particulates)
  - Liquid fragments

- Dynamic interactions of moving droplets/macroscopic particles inside the expanding vapor cloud.

- **Detail self-consistent treatments of vapor expansion, cooling, center accumulation and heating, vapor ionization and radiation cooling, and net condensation rate.**

- **Experimental data are needed on liquid (Flibe/Flinabe) properties such as vapor pressure at high temperatures, EOS, surface tension, ionization and radiation rates.**

- **Laboratory laser-liquid interaction experiments can provide very useful information.**