1. Liquid Wall Ablation
2. FLiBe Properties

A. R. Raffray and M. Zaghloul
University of California, San Diego

ARIES-IFE Meeting
Princeton Plasma Physics laboratory
Princeton, New Jersey
October 2-4, 2002

UCSD

Outline

- **Run ABLATOR for FLiBe and Pb cases to confirm simple modeling results and obtain better understanding of any integrated effect**

- **Follow up on determination of FLiBe properties**

Physical Properties for Film Materials

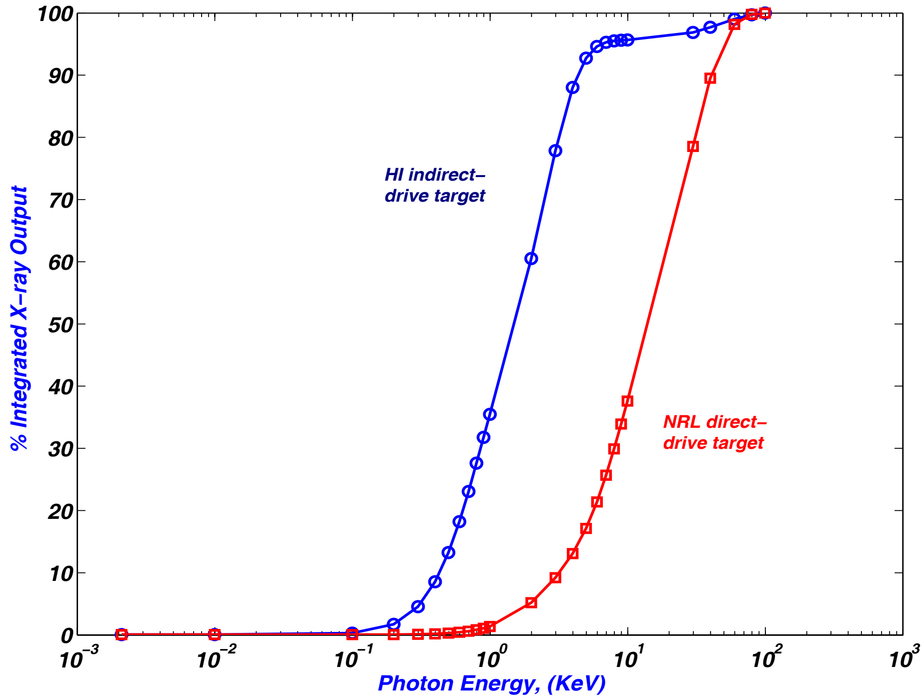
Property	Pb	FLiBe
$T_{melting}$ (K)	600.5	732.2
$T_{boiling,\ 1\ atm}$ (K)	1893	1687
$T_{critical}$ (K)	4836	4498.8 (*)
Density (kg/m^3)	11291 – 1.1647 T	2413 - 0.488 T
Vapor Pressure	$Log_{10}(P_{torr}) = 7.91 - 9923/T$	$Log_{10}(P_{torr}) = 9.38 - 10965.3/T$
C_P (J/kg-K)	$=183.6 - 0.07\ T - 1.6\times10^{6}\ T^{-2} + 3.5\times10^{-5}\ T^{2} + 5\times10^{-9}\ T^{3}$	2347
h_{fg} (J/kg)	$= 46.61 - 0.003\ T + 4.77\times10^{-7}\ T^{2}$ ($=8.6\times10^{6}$ at 1893 K)	$= 1.06\times10^{7} - 2347\ T$ (* *)

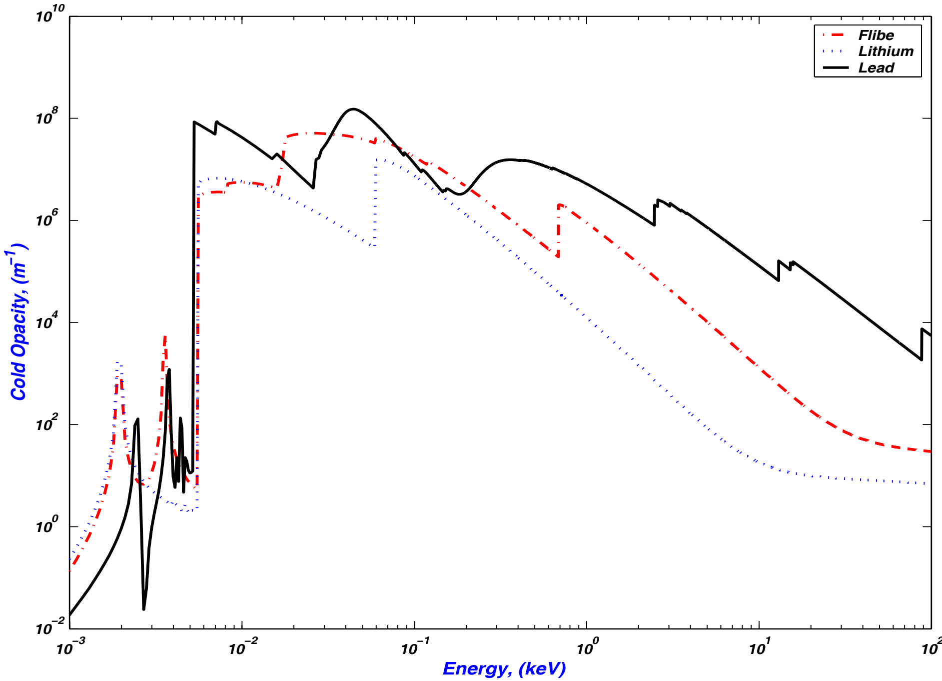
All temperatures, T, in K

(*) Xiang M. Chen, Virgil E. Schrock and Per F. Peterson, "The Soft-Sphere Equation of State for Liquid FLiBe," Fusion Technology, Vol. 21, 1992.

(**) Derived from Cp and the Cohesive energy @ 1atm.

X-ray Spectra and Cold Opacities Used in Aerosol Source Term Estimate



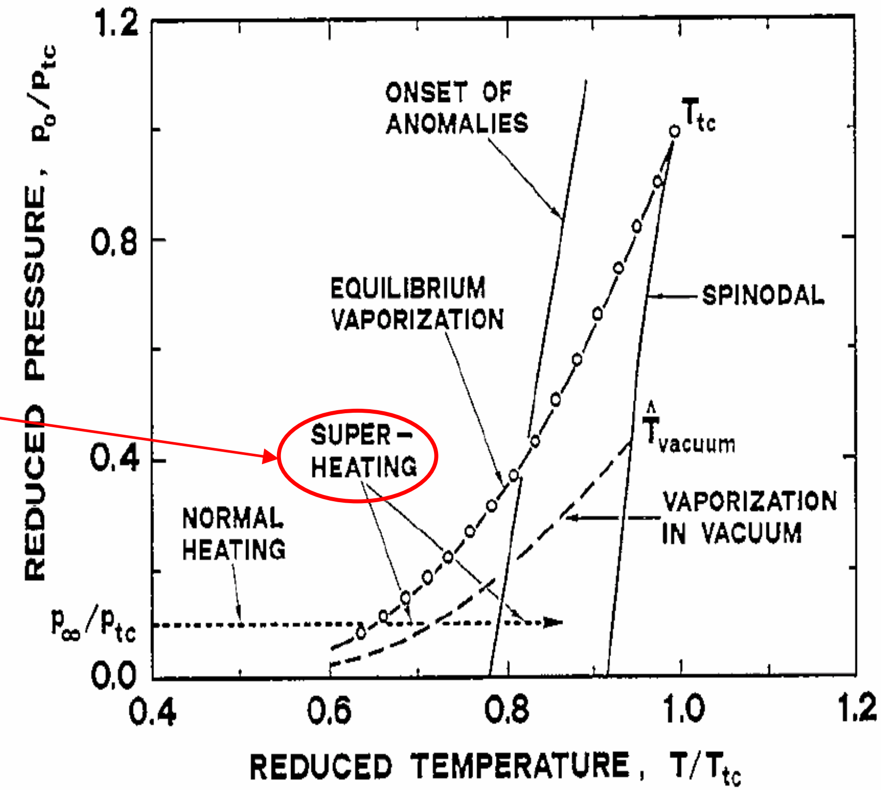


- X-ray spectra much softer for indirect drive target (90% of total energy associated with < 5 keV photons
- Cold opacity calculated from cross section data available from LLNL (EPDL97)

UCSD

Phase Explosion (Explosive Boiling)

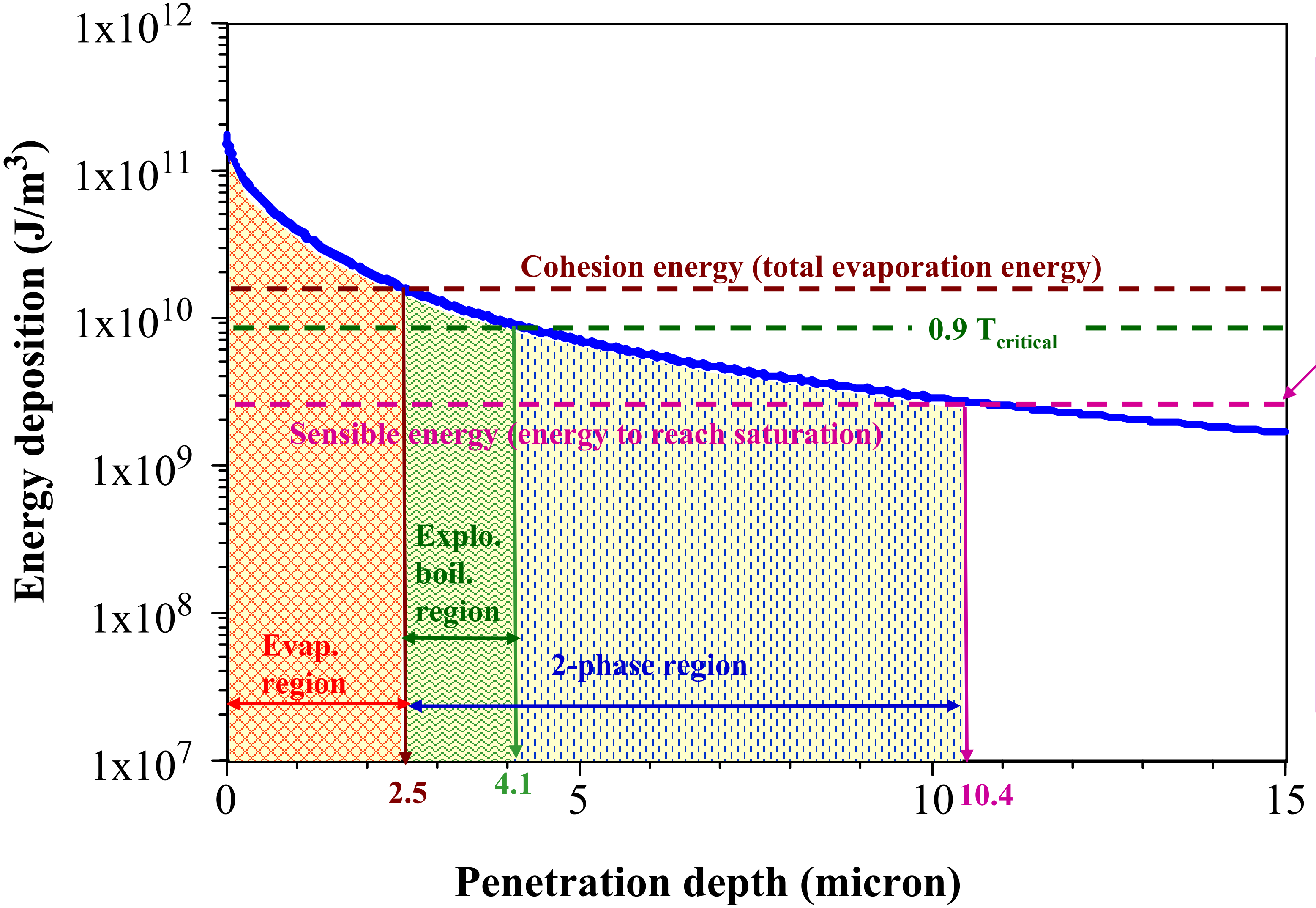
- **Rapid boiling involving homogeneous nucleation**
- **High heating rate**
  - **P_{vapor} does not build up as fast and thus falls below P_{sat} @ $T_{surface}$**
  - **superheating to a metastable liquid state**
  - **limit of superheating is the limit of thermodynamic phase stability, the spinode (defined by $\partial P/\partial v)_T = 0$)**
- **A given metastable state can be achieved in two ways:**
  - **increasing T over BP while keeping $P < P_{sat}$ (e.g. high heating rate)**
  - **reducing P from P_{sat} while keeping $T > T_{sat}$ (e.g. rarefaction wave)**



$$\frac{dN}{dt} = A\exp\left(\frac{-\Delta G_c}{kT}\right); \quad \Delta G_c = \frac{16\pi\sigma^3}{3(\rho_o h_{fg}\beta)^2}$$

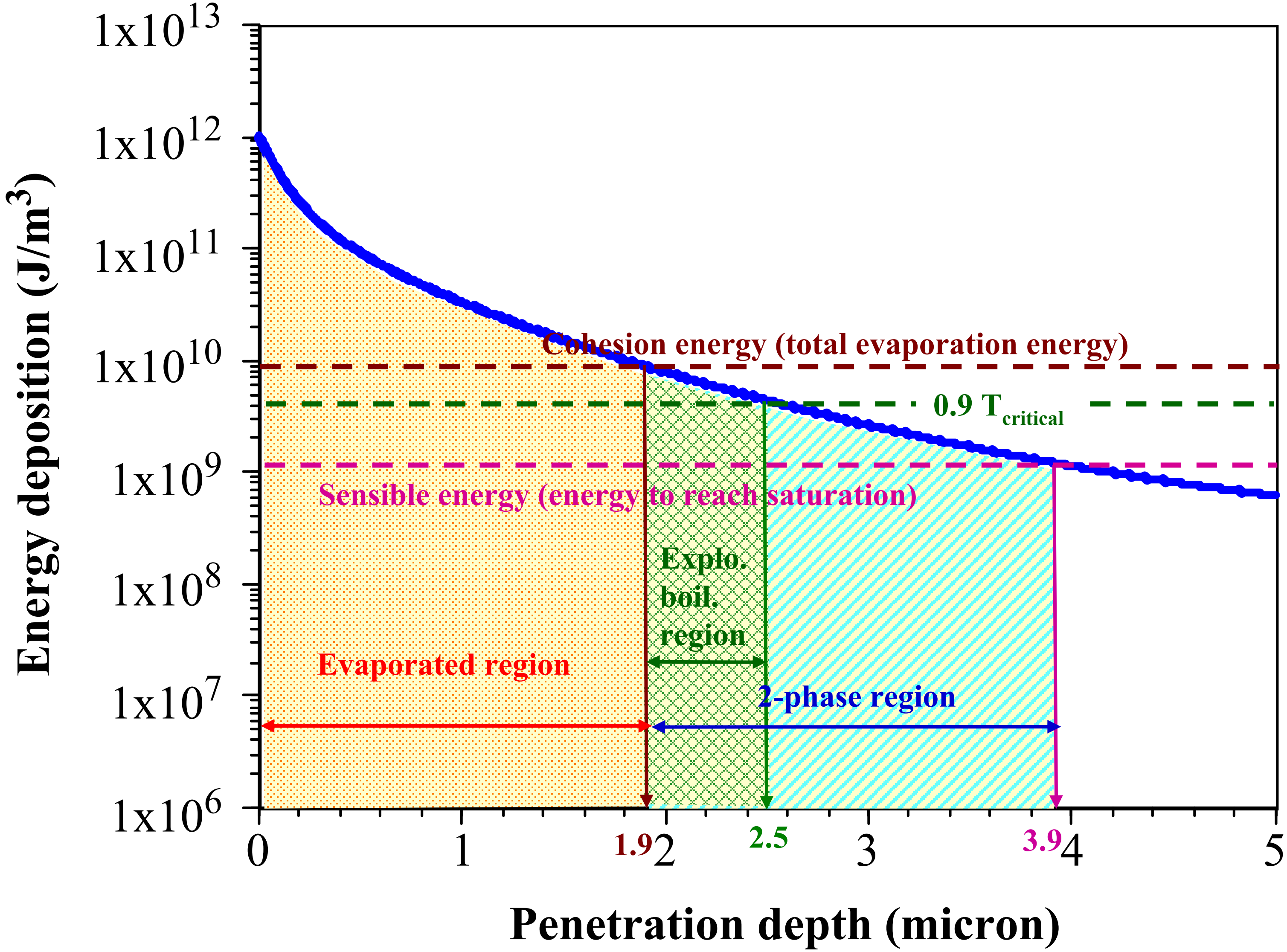
- **A metastable liquid has an excess free energy, so it decomposes explosively into liquid and vapor phases.**
  - **As $T/T_{tc} > 0.9$, Becker-Döhring theory of nucleation indicates avalanche-like and explosive growth of nucleation rate (by 20-30 orders of magnitude)**

Photon Energy Deposition Density Profile in FLiBe Film and Explosive Boiling Region



Sensible energy based on uniform vapor pressure following photon passage in chamber and including evaporated FLiBe from film

Photon Energy Deposition Density Profile in Pb Film and Explosive Boiling Region



UCSD

Summary of Results for Pb and FLiBe under the Indirect Drive Photon Threat Spectra

	Pb vapor (1 mtorr ≡ 910 K)	FLiBe vapor (1 mtorr ≡ 886 K)
$P_{vapor,interface} / P_0$	2.44×10^5	1.66×10^5
Cohesive energy, E_t (GJ/m^3)	9.14	18.02
Vapor quality in the remaining 2-phase region	0.15	0.17
$\delta_{explosive\ boil.}$ (μm)	2.46	4.07
$m_{explosive\ boil.}$ (kg)	12.89	3.96

- T_{sat} estimated from $P_{vapor,interface}$ ≡ initial vapor pressure (P_0=1 mtorr) heated by photon passage plus additional pressure due to evaporation from film based on chamber volume
- $m_{explosive,boil}$ would be lower-bound source term for chamber aerosol analysis

Processes Leading to Aerosol Formation following High Energy Deposition Over Short Time Scale

Energy Deposition & Transient Heat Transport

↓

Induced Thermal- Spikes

↓ ↓

Mechanical Response | ***Phase Transitions***

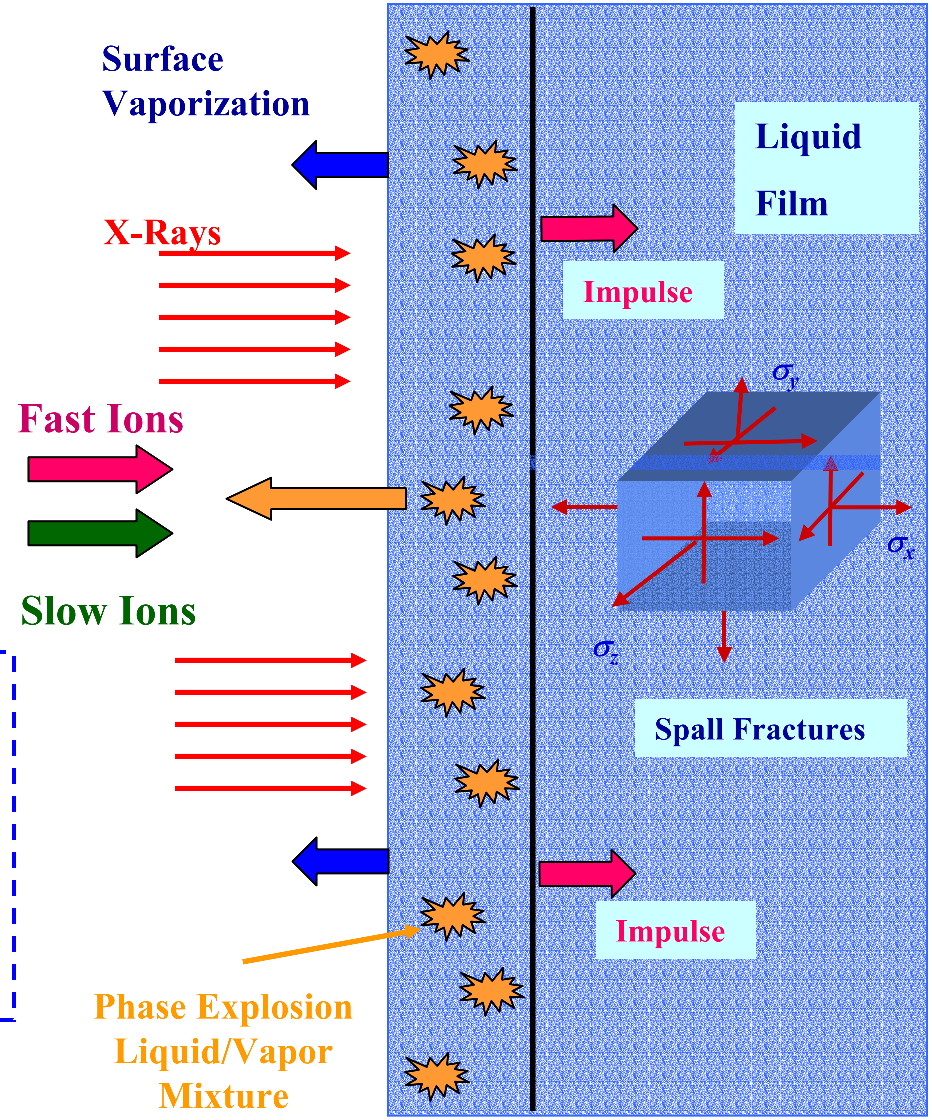
•Stresses and Strains and Hydrodynamic Motion
•Fractures and Spall

• Surface Vaporization
•Heterogeneous Nucleation
•Homogeneous Nucleation (Phase Explosion)

Material Removal Processes

↓

Expansion, Cooling and Condensation



ABLATOR Computer Model
(Ablation By Lagrangian Transient One-D Response)

Energy deposition from X-ray source (cold opacities)

- **Transient thermal conduction**
- **Thermal expansion and hydrodynamic motion**
- **Material removal mechanisms**
  - **Surface vaporization**
  - **Thermal shock/spall**
  - **Explosive boiling (homogeneous nucleation)**
- **An explicit scheme for time advancing in time**
- **Equation of state (EOS)**
  - **Gruneisen for solid and liquid**
  - **Ideal gas EOS for vapor phase**

Comparison of ABLATOR and Simple Volumetric Model Results for Lead Under 458MJ ID Photon Threat Spectra

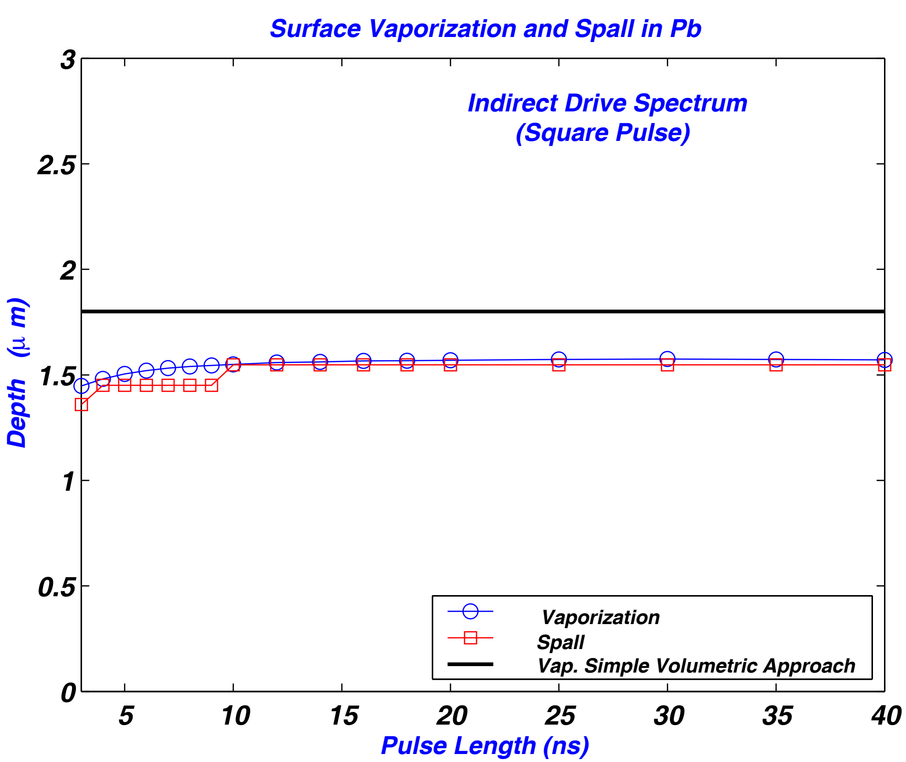
- **Surface tension**

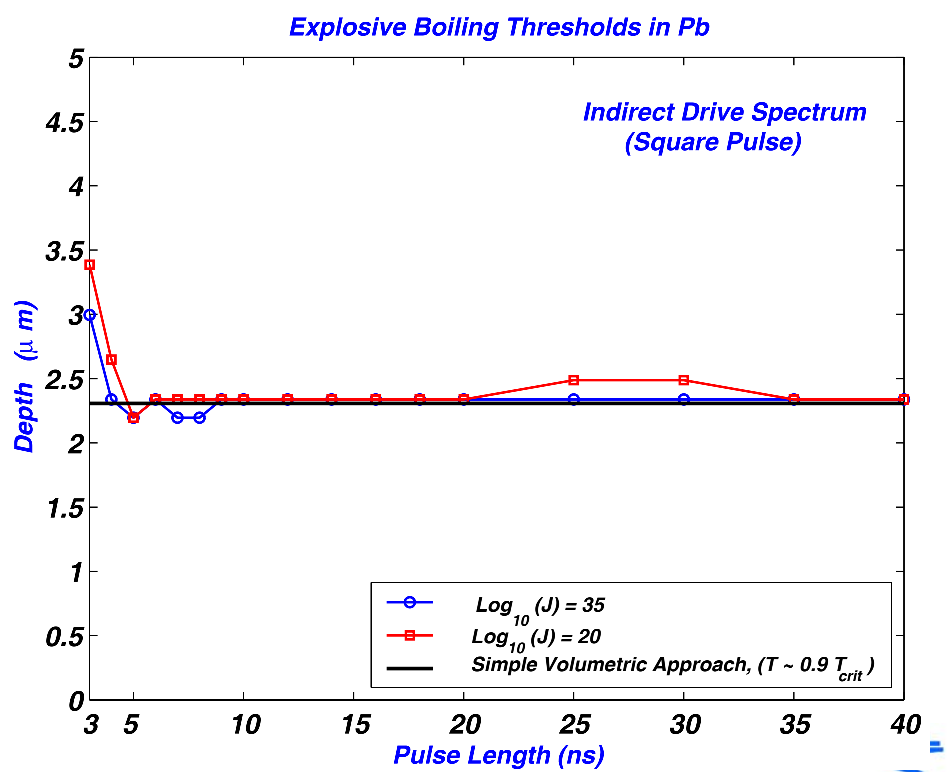
$$\sigma(N/m) = 0.444 - 9.3 \times 10^{-5}\ (T - 600.5)$$

&

$$\sigma(T_{crit} = 5374\ K) = 0.0$$

- **Enthalpy-temperature relation (JANAF tables)**
- **Theoretical tensile strength = 1.66 GPa**
- **Sound speed = 1820 (m/s)**
- **Gruneisen parameter, Γ = 2.5**





Comparison of ABLATOR and Simple Volumetric Model Results for FLiBe Under 458MJ ID Photon Threat Spectra

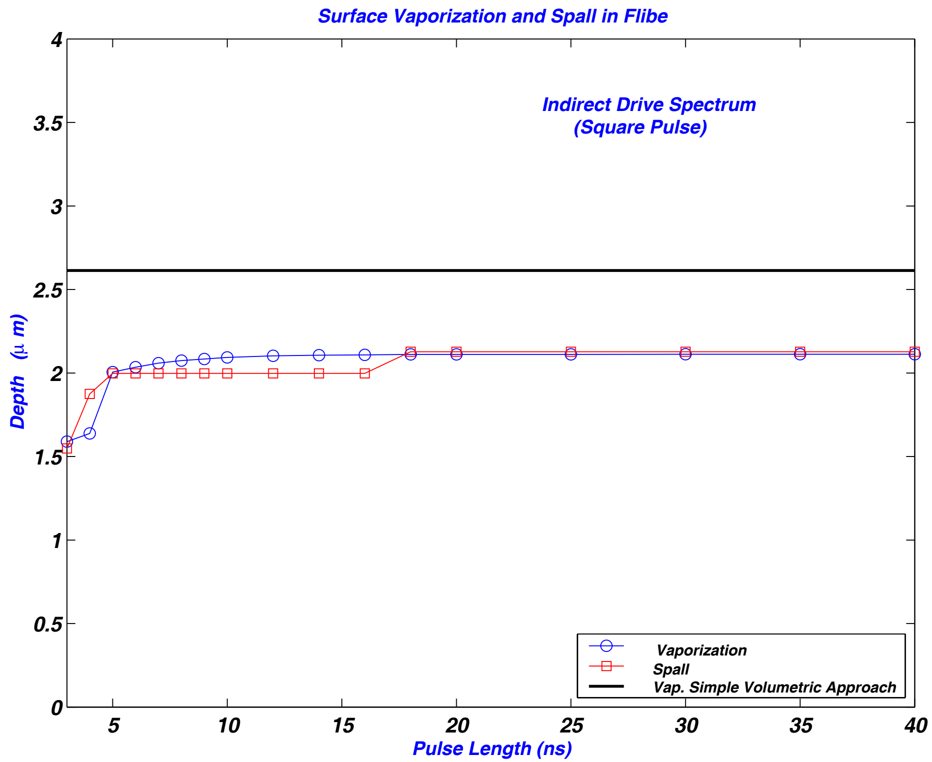
- Surface tension (linear interpolation between the value @ T_{melt} and the zero value @ T_{crit}

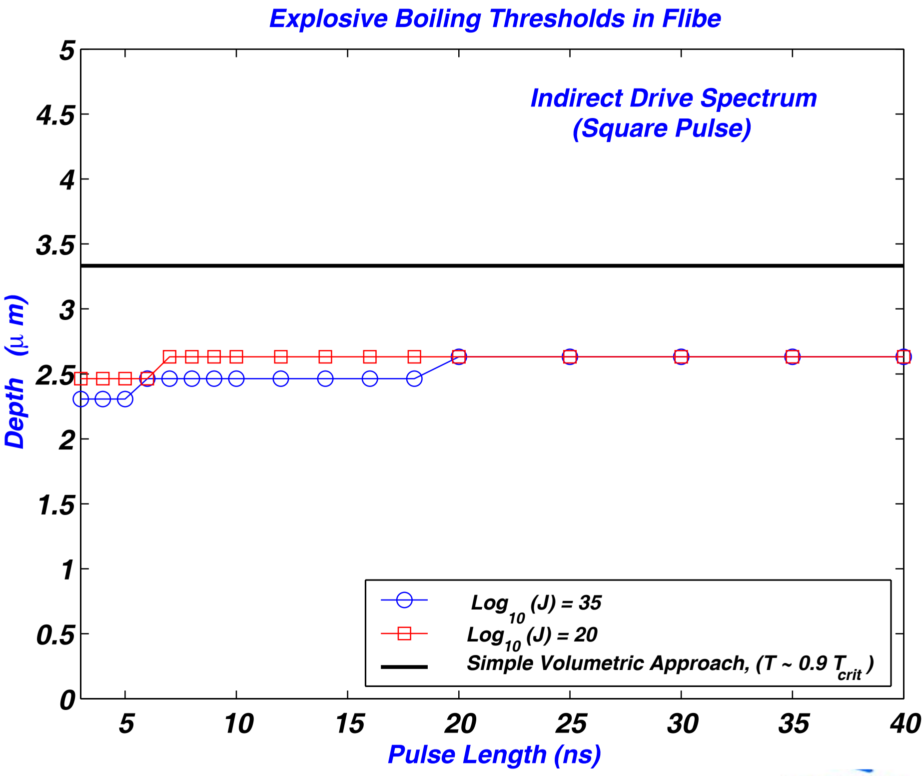
$$\sigma(N/m) = 0.207924 - 5.520350458 \times 10^{-5}\ (T - 732.3)$$

&

$$\sigma(T_{crit} = 4498.8\ K) = 0.0$$

- Enthalpy-temperature relation (JANAF tables for solid or liquid and fully dissociated ideal gas for vapor)
- Theoretical tensile strength = 0.42 Gpa
- Sound speed = 3420 (m/s)
- Gruneisen parameter, $\Gamma = 0.96$





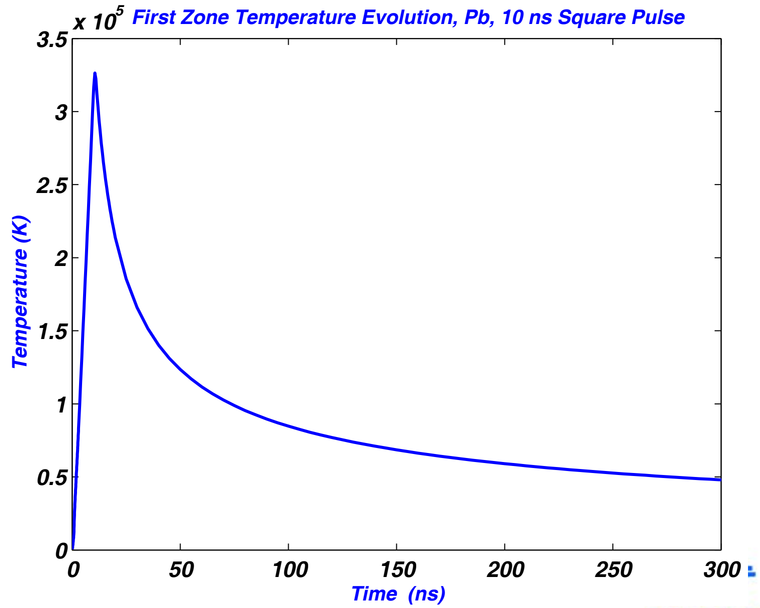
Observations from of ABLATOR Study

- Results from simple model agree reasonably well with ABLATOR results tending to be somewhat conservative

- This suggests that the simple model could be used for scoping analysis of aerosol source term
  - Lower bound ablated thickness based on explosive boiling
  - Upper bound ablated thickness based on 2-phase region

- Uncertainty still remains about the form of the source term (i.e vapor, liquid droplet size distribution and density...)
  - Should be part of future effort
  - ABLATOR could be a useful tool with modifications

- ABLATOR runs based on ideal gas properties
  - Results show high vapor temperature and ionization
  - Need properties for high temperature FLiBe including dissociation and ionization for more accurate analysis



UCSD

FLiBe Thermodynamic Properties Used at Present

Temperature

Liquid + Vapor

$T_{crit} \sim 4500$ K

- The Soft-Sphere Equation of State for Liquid FLiBe takes into account the dependence on ρ and T(*).

Vapor chemical decomposition of molecules

T ~ 1 eV

- Chemical equilibrium codes utilizing data from JANAF tables are used (e.g. the computer code STANJAN from Stanford Univ.)

Plasma multiple ionization

- Fitted Equations of State for Flibe Gas(**).
- Inaccuracies Include:
  - Use of Post-Jensen ionization data calculated from the Corona equilibrium (valid only for extremely low densities and very high temperatures-optically thin plasma) and show no dependence on density.
  - Post-Jensen data give no information on the individual populations needed for the internal energy computation and so further approximations have to be made.
  - No Coulomb corrections.
  - No excitation energies included in the computations of internal energies.

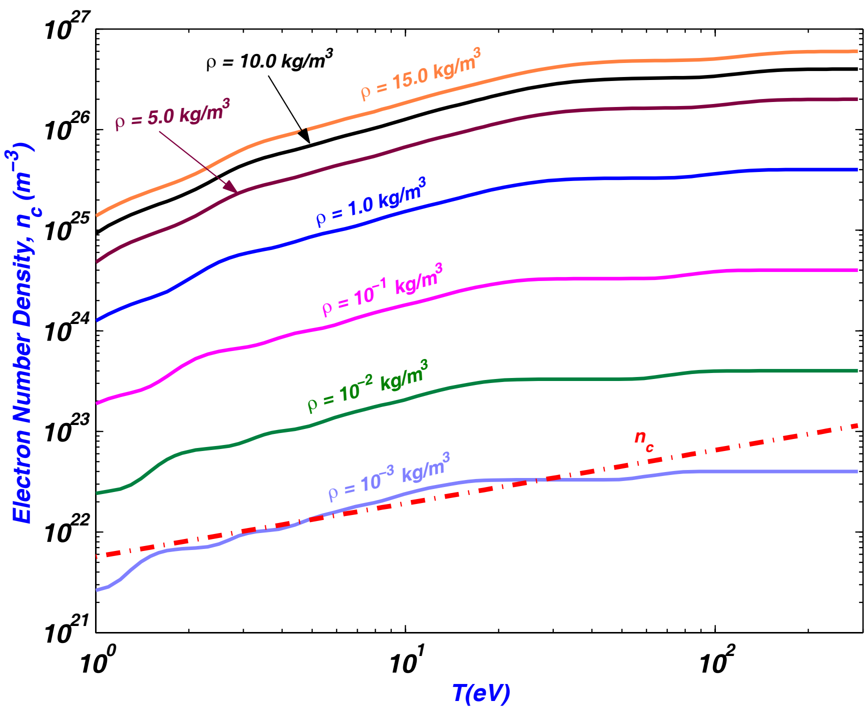
Calculations of more accurate FLiBe thermodynamic properties at high Temp.

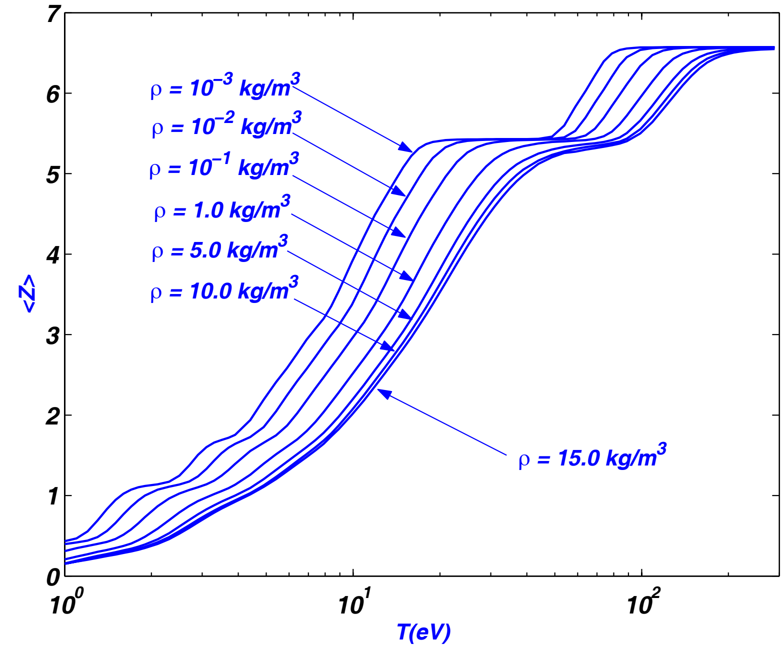
(*) Xiang M. Chen , Virgil E. Schrock, and Per F. Peterson " The soft-sphere equation of state for liquid Flibe," Fusion Tech. 21, 1525 (1992).

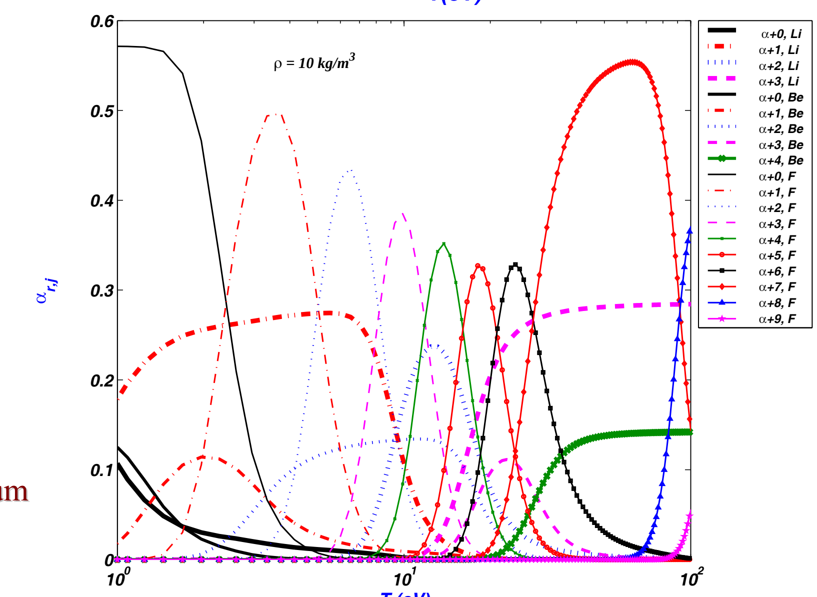
(**) Xiang M. Chen, Virgil E. Schrock, and Per F. Peterson, "Fitted Equation of State for Flibe Gas," Fusion Technology 26, 912 (1994).

Ionization Equilibrium & Validity of LTE Assumption

- Fully-Dissociated Flibe-Gas (T> 1 eV)
- LTE(local thermal equilibrium) and Electro-neutrality Assumptions
- Set of Coupled Non-linear Saha Equations with Continuum Lowering (Debye-Huckel theory with quantum mechanical finite ionic size(*))
- Criterion for LTE Assumption by Fujimoto(**)







(*) W. Ebeling et al, Theory of Bound States and Ionization Equilibrium in Plasmas and Solids (Akademic-Verlag, 1976)

(**) T. Fujimoto et al, Phys. Rev. A 42, 6588 (1990).

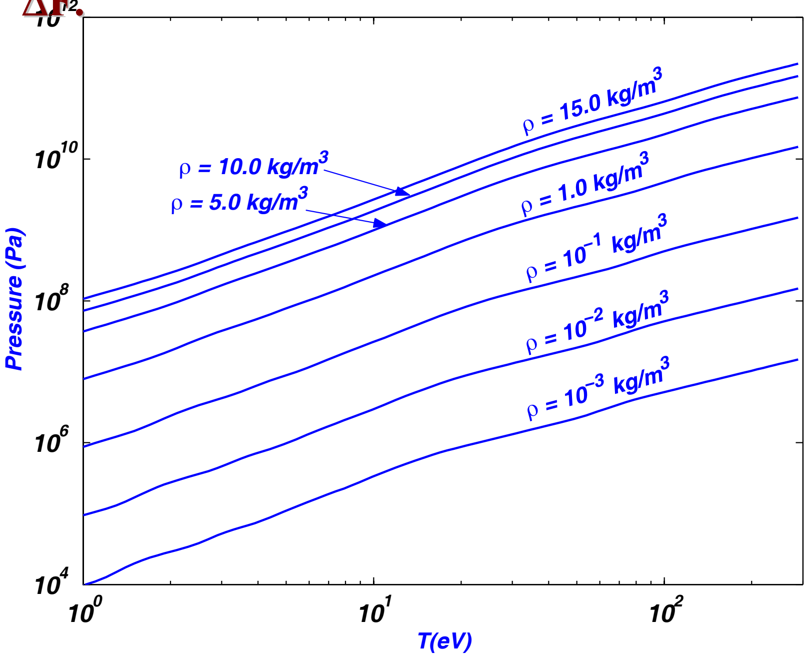
Thermodynamic Functions (Pressure and Internal Energy)

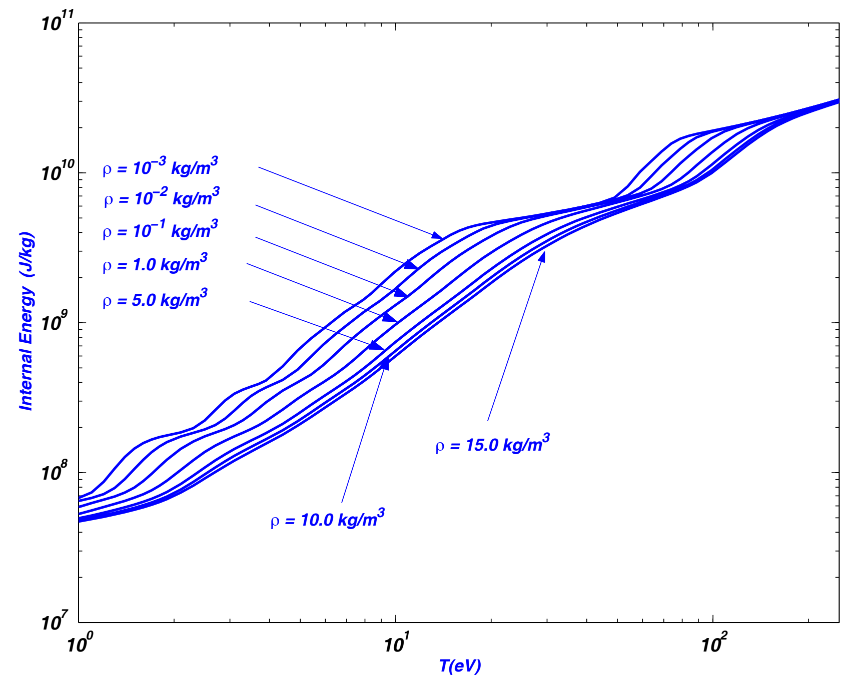
- **Chemical Model of Partially Ionized Plasma (mixture of weakly interacting electrons, ions and atoms in a constant volume).**
- **Free Energy F, with Coulomb Correction ΔF.**

$$F = F_{id} - \Delta F_{coul} = F_{id} - \frac{K_B T V}{12 \pi} \kappa^3 \tau(\kappa a)$$

$$\kappa^{-1} = \lambda_D = \left(\varepsilon_0 K_B T \Big/ e^2 \left(n_e + \sum_{j=1}^{J} \sum_{i=0}^{Z_{max,j}} z_i^2 n_i \right) \right)^{1/2}$$

$$\tau(\chi) = \frac{3}{\chi^3} \left[\ln(1+\chi) - \chi + \frac{\chi^2}{2} \right]$$





$$P = n_H K_B T (1 + \bar{Z}_{av}) + \Delta P_{Ccoul}$$

$$e = \frac{1}{\rho} \left(\frac{3}{2} n_H (1 + \bar{Z}_{av}) K_B (T - T_0) + n_H \sum_{j=1}^{J} \sum_{i=1}^{Z_{max,j}} \alpha_i \left(\sum_{z=1}^{i} (I_z - \Delta I_z) + W_{j,i} \right) + \Delta E_{Coul} \right)$$

Thermodynamic Functions (cont.)
Enthalpy, Specific Heat, Adiabatic Exponent and Sound Speed

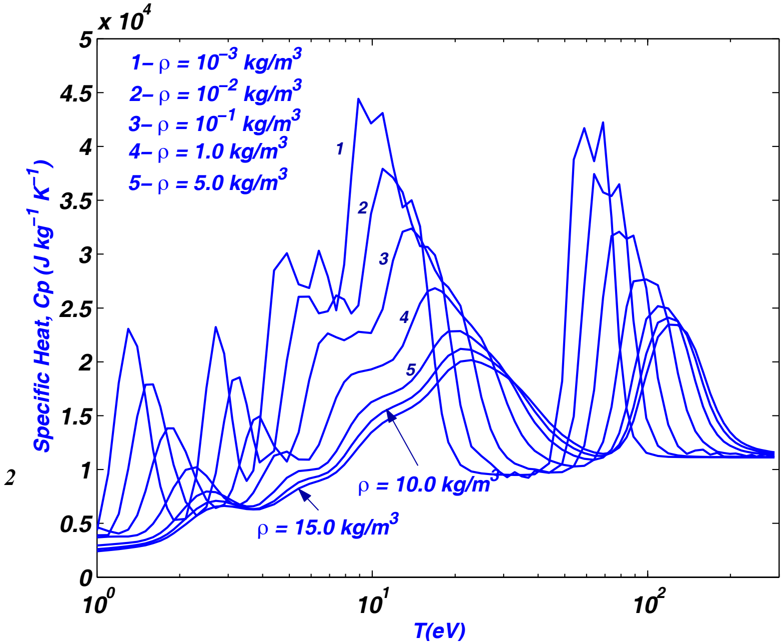
- **Enthalpy**

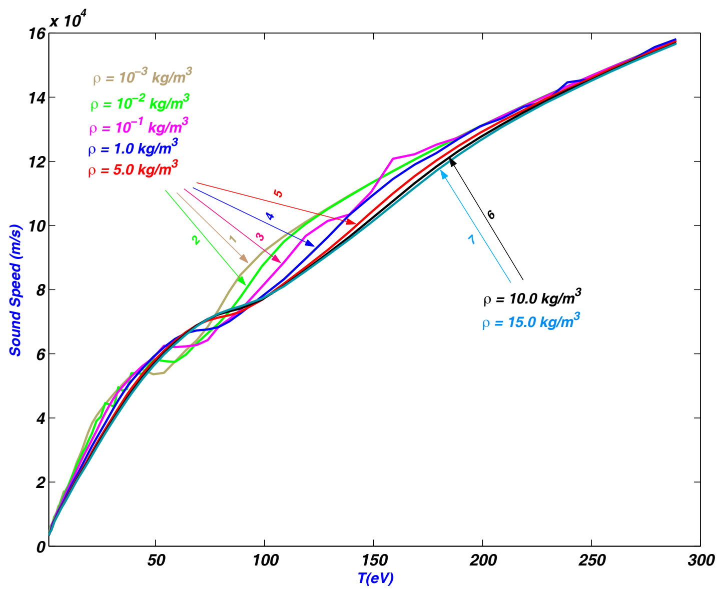
$$h_e = \frac{1}{\rho}(\rho e + P)$$

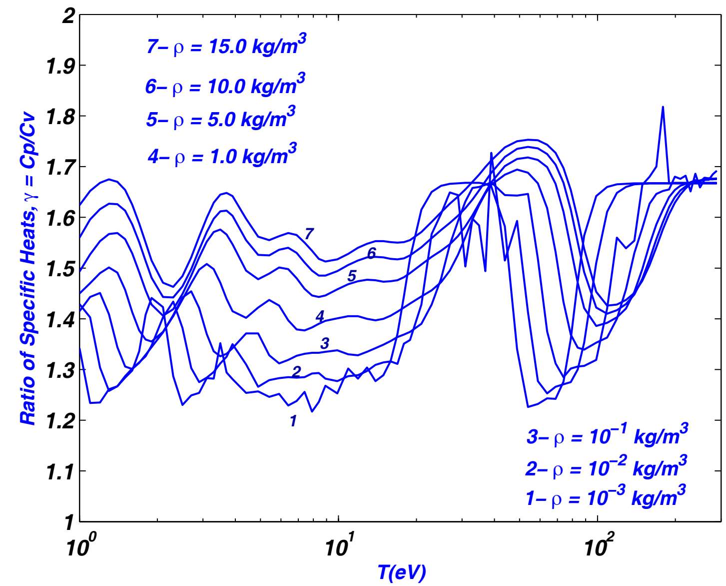
- **Most Rigorous Expressions for Cp, γ, and Sound Speed**

$$C_v = (\partial e / \partial T)_{1/\rho}, \quad C_P = (\partial h_e / \partial T)_P,$$

$$\gamma = C_P / C_v, \text{ and } \quad v_s = \left(\frac{\partial P}{\partial \rho}\right)_S^{1/2} = \left[\gamma \left(\frac{\partial P}{\partial \rho}\right)_T\right]^{1/2}$$



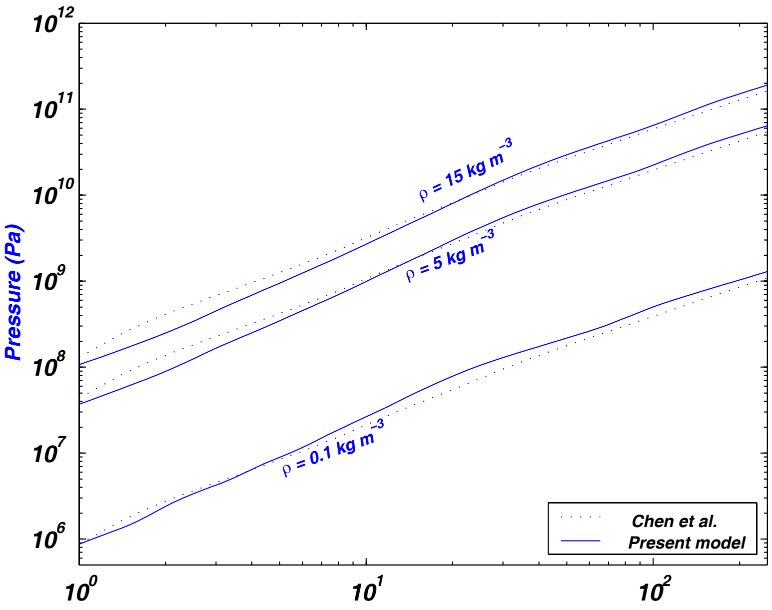


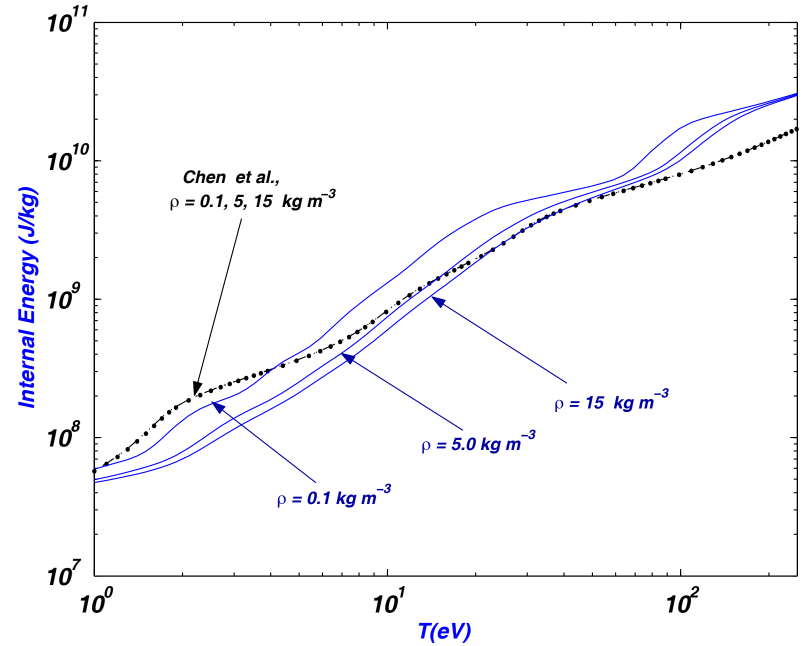


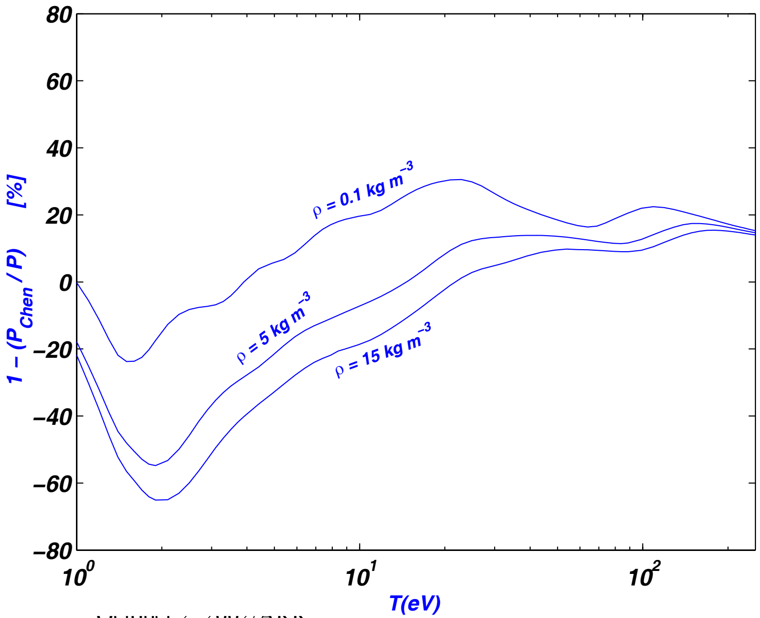
CSD

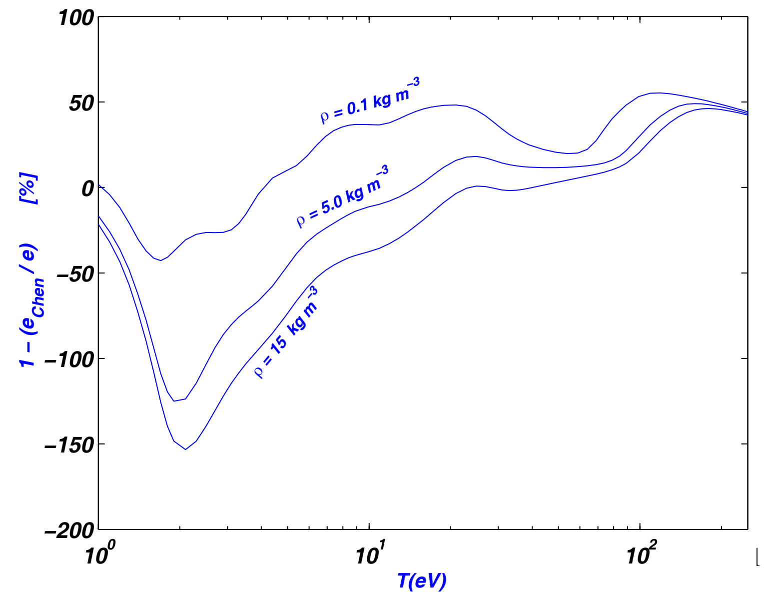
Comparison with Results from Chen et al.,(*)

(*) Xiang M. Chen, Virgil E. Schrock, and Per F. Peterson, Fusion Technology 26, 912 (1994).









Comparison of Newly Derived High Temperature FLiBe Properties with Chen's Derivations

- Up to ~65% difference between Chen's and the new derivation for pressure and ~150% for internal energy

- Property data available for use by others

- Need to modify ABLATOR to utilize new data and to run cases

Summary Slide on Future Effort

- Need better characterization of aerosol source term in terms of vapor/liquid characteristics of ejecta (ARIES/UCSD,...)
  - Better understanding of explosive boiling, other ablation mechanisms (spalling) to estimate form of expelled vapor/liquid
  - Can be based on ABLATOR with modifications

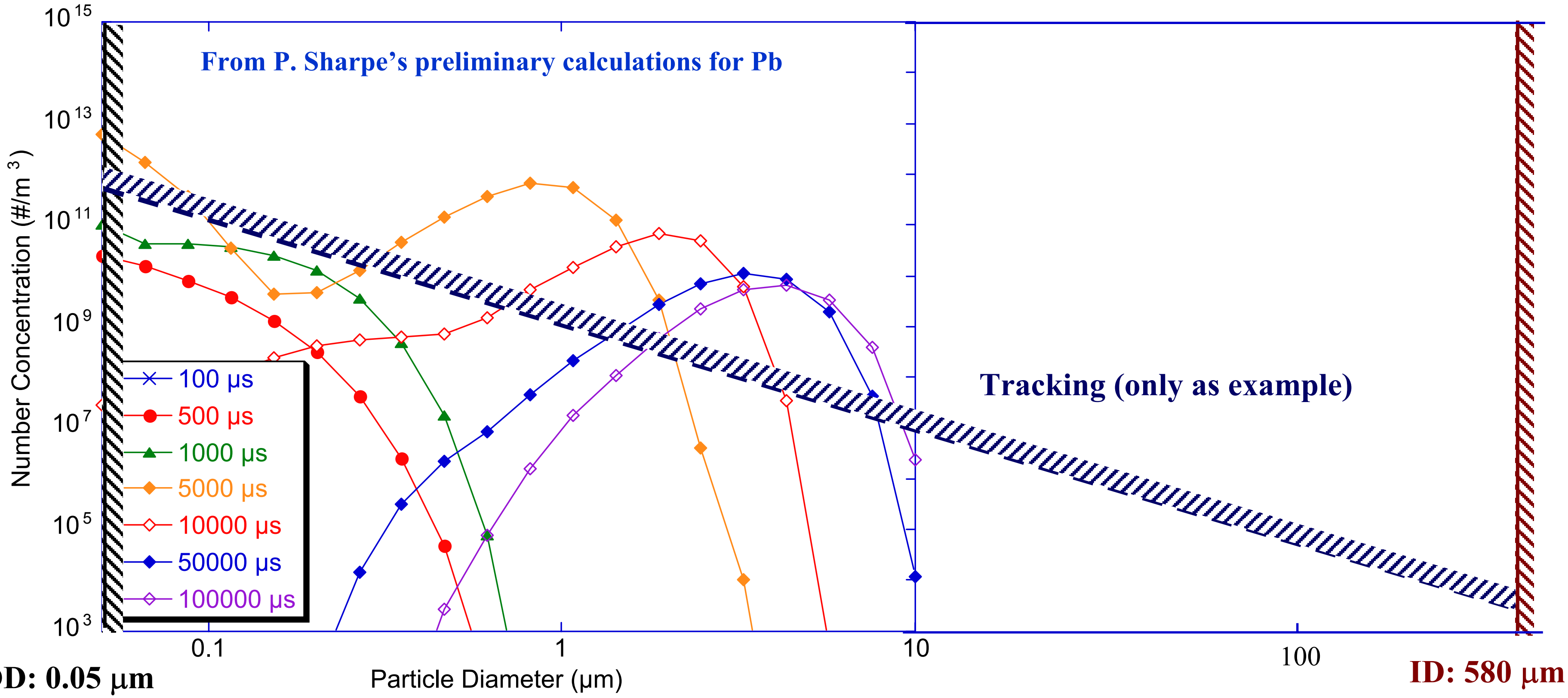
- Need experiments to measure amount of ablated material and form of ejecta for better understanding and for model validation (IFE program)
  - Explosive boiling can be simulated by laser/material interaction experiment (similar heating rate)

- Need more detailed aerosol modeling in chamber (ARIES/INEEL, UCSD,….)
  - More accurate model for FLiBe
  - More accurate source term including initial cooling down of plasma to state at threshold of nucleation

- Need experiments to simulate aerosol formation and transport for better understanding and for code validation (IFE program)

Example Aerosol Operating Parameter Window

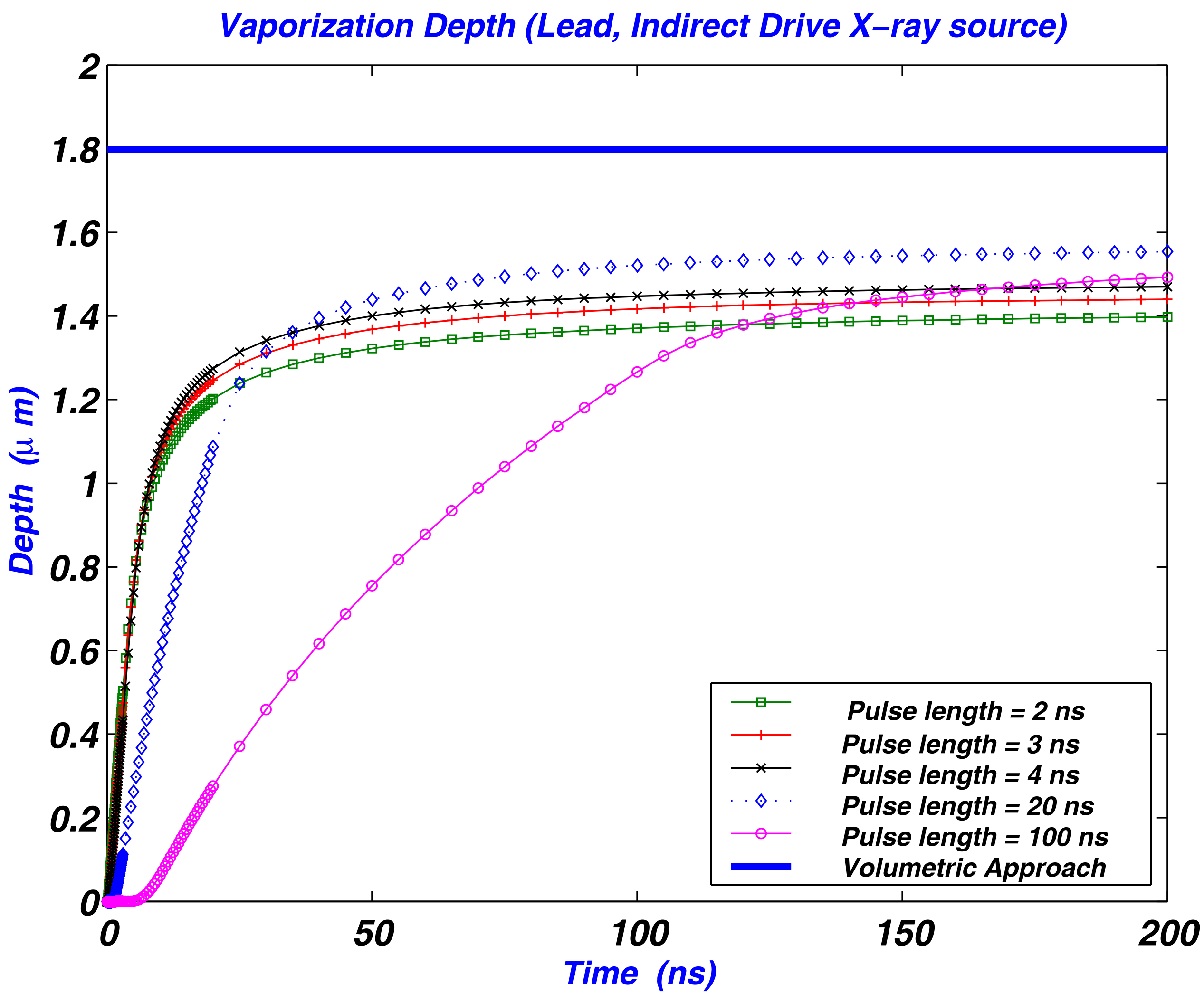
- **Use explosive boiling results as input for aerosol calculations**
- **Perform aerosol analysis to obtain droplet concentration and sizes prior to next shot (NOT DONE YET)**
- **Apply target and driver constraints (e.g. from R. Petzoldt)**



- **Need aerosol analysis for explosive boiling source case for Pb and FLiBe**
- **Need target tracking constraints for FLiBe**
- **Need to finalize driver constraints on aerosol size and distribution**

Extra Slide

Example of ABLATOR Results



UCSD