Modeling and Simulations of Cavitating and Bubbly Flows

Roman Samulyak
Tianshi Lu, Yarema Prykarpatskyy

Center for Data Intensive Computing
Brookhaven National Laboratory
U.S. Department of Energy

rosamu@bnl.gov
Talk Outline

- Two approaches to the modeling of cavitating and bubbly fluids:
  - Homogeneous Method (homogeneous equation of state models)
  - Direct Method (direct numerical simulation)

- Simulations of targetry experiments obtained with Homogeneous Method

- Benchmark problems for the Direct Method: simulation of classical experiments on waves in bubbly fluids

- Some applications of the Direct Method to SNS target problems

- Simulations of the mercury jet interacting with proton pulses

- Conclusions and future plans
Previous simulations with one-phase fluid EOS.

Mercury jet evolution due to the proton pulse energy deposition

$E_{\text{max}} = 100 \text{ J/g, } B = 0$

a) Initial shape of the jet, $t = 0$;  
b) Instabilities due to the second reflected shock wave, $t = 40$  
c) Interaction of the third reflected shock wave with the surface, $t = 90$  
d) Instabilities due to the third reflected shock wave, $t = 59$;  
e) Interaction of the fourth reflected shock wave with the surface, $t = 67$. 
Previous simulations with one-phase fluid EOS

Positive features

• Qualitatively correct evolution of the jet surface due to the proton energy deposition

Negative features

• Discrepancy of the time scale with experiments
• Absence of cavitation in mercury
• The growth of surface instabilities due to unphysical oscillations

Conclusion

• Cavitation is very important in the process of jet disintegration
• There is a need for cavitation models/libraries to the FronTier code
EOS for cavitating and bubbly fluids: two approaches

- **Direct method**: Each individual bubble is explicitly resolved using FronTier interface tracking technique.

  - Stiffened polytropic EOS for liquid
  - Polytropic EOS for gas (vapor)

- **Homogeneous EOS model**: Suitable average properties are determined and the mixture is treated as a pseudofluid that obeys an equation of single-component flow.
Direct method: Pro and Contra

Advantages:
- Accurate description of multiphase systems limited only to numerical errors.
- Accurate treatment of drag, surface tension, viscous, and thermal effects. More easy to account for the mass transfer due to phase transition.
- Discontinuities of physical properties are also beneficial for MHD.

Disadvantages:
- Very complex and computationally expensive, especially in 3D.
- Designed only for FronTier. Impossible to create a general purpose EOS library.
Example: Isentropic EOS model for two-phase fluids

- The most important feature is correct dependence of the sound speed on the density (void fraction).

- Enough input parameters (thermodynamic/acoustic parameters of both saturated points) to fit the sound speed to experimental data.

- Absence of drag, surface tension, and viscous forces. Incomplete thermodynamics (isentropic approximation). No features of bubble dynamics.

- Despite simplicity, the EOS led to significant improvements (of the time scale) in modeling of the mercury – proton pulse interaction.
Numerical simulation of the interaction of a free mercury jet with high energy proton pulses using two phase EOS

Evolution of the mercury jet after the interaction with a proton pulse during 1.2 ms.
Mercury thimble experiment at AGS (BNL)

Left: picture of the experimental device
Right: schematic of the thimble in the steel bar
Mercury splash (thimble): experimental data

Mercury splash at $t = 0.88$, 1.25 and 7 ms after proton impact of 3.7 $e12$ protons
Mercury splash (thimble): numerical simulation

$I = 3.7 \times 10^{12} \text{ protons / pulse}$

$t = 240 \mu s \quad t = 480 \mu s \quad t = 609 \mu s \quad t = 1.014 ms$
Mercury splash (thimble): numerical simulation

\[ E = 17 \times 10^{12} \text{ protons / pulse} \]

\[ t = 200 \mu s \quad t = 515 \mu s \quad t = 810 \mu s \quad t = 1.2 ms \]
Velocity as a function of the r.m.s. spot size
Conclusions

- Numerical simulations show a good agreement with experimental data (especially at early time).

- The lack of full thermodynamics in the EOS leads to some disagreements with experiments for the time evolution of the velocity during several microseconds.

  Experimental data on the evolution of the explosion velocity (from Adrian Fabich’s thesis)

- Equation of states needs additional physics (bubble dynamics, mass transfer, surface tension, viscosity etc.).
EOS models based on Rayleigh-Plesset equation

A dynamic closure for fluid dynamic equations can be obtained using Rayleigh-Plesset type equations for the evolution of an average bubble size distribution

\[
R \frac{d^2 R}{dt^2} + \frac{3}{2} \left( \frac{dR}{dt} \right)^2 + \frac{4 \nu_L}{R} \frac{dR}{dt} + \frac{2S}{\rho_L R} \frac{dR}{dt} = \frac{P_B - P_L}{\rho_L}
\]

\[
\rho = \rho_L (1 - \beta) + \rho_g \beta \approx \rho_L (1 - n \cdot \frac{4}{3} \pi R^3)
\]

\[
P_B R^{3\gamma} = \text{Const.}
\]

- EOS includes implicitly drag, surface tension, and viscous forces.
Direct numerical simulations using Front Tracking.

I. Bubbly fluids (non-dissolvable gas bubbles)

Computational domain:
Region around a long column of bubbles

Approximations:
- The pressure field is assumed to be axisymmetric.
- The influence from the neighboring bubbles can be approximated by the Neumann boundary condition on the domain wall.
Propagation of Linear Waves

Entire domain of computation

Magnified view of the first 4 bubble layer

Bubbly region

$t = 0$
$t = 0$
$t = 0.005\text{ms}$
$t = 0.01\text{ms}$
$t = 0.05\text{ms}$
Linear Wave Propagation

- $R = 0.12 \text{ mm}, \ b = 2.0E-4, \ P = 1.0 \text{ bar}$.
- The amplitude of the incident pressure wave is 0.1 bar. Linearity has been checked by comparison with pressure wave of amplitude 0.05 bar.
- Grid size is $90 \times 10800$ (bubble diameter is 12 grids). Mesh refinement has been carried out and gave essentially the same result.
- The resonant frequency is
  \[
  \frac{1}{2\pi} \frac{1}{R} \sqrt{\frac{3\gamma P}{\rho_l}} = 27.2 \text{kHz}
  \]
- Sound speed measurement near resonant frequency has large error due to the strong attenuation.
Dispersion relation for linear waves

Theor y with $\delta=0.5$

Theor y with $\delta=1$

Simulation results

$c$ (m/s)

$f$ (kHz)
Attenuation of linear waves

Simulation results
Theory with $\delta=0.5$
Theory with $\delta=1$

$\alpha$ (dB/cm)
f (kHz)
1) Oscillation amplitude is smaller for gas with larger $\gamma$.

2) The simulation results agree with the experiments of Beylich & Gülhan (1990) qualitatively.

3) The oscillation periods shown in the figure differ from the experimental data by 10% to 20%.

4) The oscillation amplitudes are considerably smaller than in the experiments, which could be cured partly by mesh refinement.

$P_a = 1.1$ atm, $P_b = 1.727$ atm, $R = 1.18$ mm, $\beta = 2.5E-3$

Measured 40 cm from the interface.

Grid size is 35×7000. (Bubble diameter is 12 grids.)
Beylich & Gülhan’s experiment

Simulation results
Comments on the Simulations

Viscosity

Not important in both linear and shock wave propagations.

Surface tension

Only important for bubbles with diameter of the order of 1\(\mu\)m.

Heat conduction

Several authors, e.g., Watanabe & Prosperetti (1994), claimed that heat conduction is crucial in the propagation of shock wave. We will discuss it together with phase transition between the bubbles and the fluid.
Application to SNS target problem

Cavitation induced pitting of the target flange

Courtesy of Oak Ridge National Laboratory
Pressure evolution

Pure mercury

\[ P_0 = 500 \text{ bar} \quad \text{First } P_{\min} = -150 \text{ bar at } 16 \, \mu\text{s}. \]

Mercury with air bubbles

\[ R = 1.0 \, \text{mm}, \, \beta = 2.5\% \]

\[ P_0 = 500 \text{ bar} \quad \text{First } P_{\min} = -540 \text{ bar at } 6 \, \mu\text{s}. \]
Effects of bubble injection:

- Peak pressure decreases by several times.
- Minimum pressure (negative) has larger absolute value.
- Cavitation lasts for a short time.
Cavitation bubble evolution.
Top: radius, Bottom: velocity

\[ P_{\text{max}} = -200 \text{ bar} \]
\[ t = 10 \text{ microseconds} \]

\[ P_{\text{max}} = -500 \text{ bar} \]
\[ t = 10 \text{ microseconds} \]

\[ P_{\text{max}} = -300 \text{ bar} \]
\[ t = 40 \text{ microseconds} \]
Dynamic cavitation

- A cavitation bubble is dynamically inserted in the center of a rarefaction wave of critical strength.
- A bubble is dynamically destroyed when the radius becomes smaller than critical. “Critical” radius is determined by the numerical resolution, not the surface tension and pressure.
- There is no data on the distribution of nucleation centers for mercury at the given conditions. Theoretical estimates usually disagree with experiments.

\[
R_C = \frac{2S}{\Delta P_C} \quad \text{critical radius}
\]

\[
J = J_0 e^{-Gb}, \quad J_0 = N \sqrt{\frac{2S}{\pi m}}, \quad Gb = \frac{W_{CR}}{kT}, \quad W_{CR} = \frac{16\pi S^3}{3(\Delta P_C)^2}
\]

nucleation rate
II. Dynamic cavitation

- There are uncertainties in the initial states before cavitation
- Numerical resolution is very important and the local mesh refinement is critical for achieving high quality results
- Adaptive mesh refinement (AMR) library has been developed for the FronTier code. At this moment, does not work with the dynamic cavitation.

Example of the AMR in FronTier: high speed fuel jet breakup.
Cavitation in the mercury jet. Energy deposition is 80 J/g.
Velocity of the jet surface as a function of the energy deposition
Conclusions and Future Plans

- Two approaches to the modeling of cavitating and bubbly fluids have been developed
  - Homogeneous Method (homogeneous equation of state models)
  - Direct Method (direct numerical simulation)

- Simulations of linear and shock waves in bubbly fluids and the interaction of mercury jet and thimble with proton pulses have been performed and compared with experiments.

- Both directions are promising. Future developments:
  - Homogeneous method: EOS based on the Rayleigh–Plesset equation.
  - Direct numerical simulations: AMR, improvement of thermodynamics, mass transfer due to the phase transition.
  - Continue simulations of hydro and MHD processes in the mercury target.