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Title: Formulation of a multifluid mix model with strength effects

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Formulation of a multifluid mix model with strength effects (U)

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Abstract

Including strength effect implies that mixing materials are segregated in small scales. We thus chose the multiphase form of multifluid models, since it provides the proper form of pressure forces for segregated material. The pressure term has been extended for multi-pressure cases, providing the correct physical description of segregated materials. Multi-pressure models also alleviate numerical difficulty encountered in single-pressure models. Ensemble averaging of the pressure term leads to a contact force term. Using conservation of unresolved kinetic energy (UKE), we can derive a functional form of this contact force, resulting in the well-known virtual mass term. The virtual mass coefficient can be obtained in special cases of Rayleigh-Taylor and Richtmyer-Meshkov instabilities, using an ordinary differential equation (ODE) model which can be interpreted as a representation of experimental data in a differential equation form. Strength effects are included by generalizing pressure force to include deviatoric stress, which requires mesh resolution of interfaces. Therefore, subzonal strength effects are represented by an additional term. The functional form and coefficients are obtained by using an ODE model in a similar manner used in closing the virtual mass coefficient. The virtual mass force coefficient is consistent with the small-scale strength in the linear growth regime. (U)

Formulation of a multifluid mix model with strength effects

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LANL

JOWOG32P Meeting, May 16-20, 2011

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Outline

- **Pressure force term**
  - Different from the AJS model
  - Strength
  - Contact force
- **Virtual mass force from contact force**
- **Virtual mass coefficient**
- **Drag coefficient**
- **Subzonal scale strength effects**
- **Implementation underway**

Multicomponent and multiphase mixtures

- **There are essentially two types of mixtures**
  - Mixed at molecular level – multicomponent
  - Physically separate in small scales – multiphase
- **Species momentum equations take similar forms**

$$\frac{\partial \alpha_i \rho_i \mathbf{u}_i}{\partial t} + \nabla \cdot \left(\alpha_i \rho_i \mathbf{u}_i \mathbf{u}_i \right) = \mathbf{G}_i + \mathbf{F}_i + \mathbf{V}_i + \mathbf{T}_i$$

- **The driving force $\mathbf{G}_i$ takes the form**

$$\mathbf{G}_i = -\alpha_i \nabla p \quad \text{for multiphase fluid flow}$$

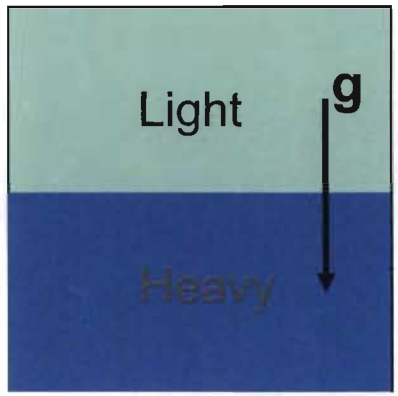
$$\mathbf{G}_i = -\nabla p_i = -\nabla(\alpha_i p) \quad \text{for multicomponent fluid flow}$$

- **The main difference between these two limiting cases is that the volume fraction is inside the gradient in multi-component mixtures, while outside in multi-phase mixtures.**

This seemingly simple difference has profound effects

- **These two limiting cases are physically quite different.**

Driving force due to $\nabla \alpha_i p$ is non-zero, resulting in mixing (diffusion).



Driving force due to $\alpha_i \nabla p$ is zero, resulting in no mixing.

- **Multicomponent momentum equations are stable and well-behaved.**
- **Multiphase flow equations are ill-posed and unstable in the absence of regularizing effects (viscous stress, surface tension, numerical viscosity, etc.)**

We chose the multiphase equations

- **Physical characteristics**
  - Separated in small scales
  - Inertial effects (e.g., demixing)
- **Multiphase equation can be derived by averaging over statistical fluid element distribution**
  - Materials separate at small scales, leading to multiphase model
  - Results similar to Youngs' model

$$\left\langle X_i \left[\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) = -\nabla p \right] \right\rangle$$

$$X_i = \begin{cases} 1 & \text{when material } i \text{ is present} \\ 0 & \text{when material } i \text{ is absent} \end{cases}$$

- **Resulting in**

$$\alpha_i \rho_i \left(\frac{\partial \mathbf{u}_i}{\partial t} + \mathbf{u}_i \cdot \nabla \mathbf{u}_i \right) = -\langle X_i \nabla p \rangle + \nabla \cdot (\alpha_i \mathbf{S}_i)$$

Resulting multiphase model

$$\alpha_i \rho_i \left(\frac{\partial \mathbf{u}_i}{\partial t} + \mathbf{u}_i \cdot \nabla \mathbf{u}_i \right) = -\langle X_i \nabla p \rangle + \nabla \cdot (\alpha_i \mathbf{S}_i) + \mathbf{T}_i + \sum_j \mathbf{F}_{ij} + \alpha_i \rho_i \mathbf{g}$$

- **Stress (force) field represented for each fluid, including $\mathbf{S}_i$.**
  - Natural framework for pressure nonequilibrium
  - Strength added by replacing $\mathbf{S}_i$ with deviatoric stress
  - Turbulence can be included by adding Reynolds stress to $\mathbf{S}_i$
- **Automatic representation of inertial difference between mixing materials**
  - Instabilities
  - Demixing
- **Compared to single-fluid turbulence modeling, different set of terms need to be closed.**
  - No natural separation of length scales – DNS difficult, perhaps impossible.

Closing of the pressure term

$$-\langle X_i \nabla p \rangle = -\alpha_i \nabla \overline{p} - \nabla\left[\alpha_i \left(p_i - \overline{p}\right)\right] + \left\langle \left(p - \overline{p}\right) \nabla X_i \right\rangle$$

$$\alpha_i p_i = \langle X_i p \rangle$$

$$\overline{p} = \langle p \rangle = \sum_i \alpha_i p_i$$

$-\alpha_i \nabla \overline{p}$ — Mean net force per unit volume exerted by $\overline{p}$ on phase *i*

$-\nabla\left[\alpha_i \left(p_i - \overline{p}\right)\right]$ — Force due to deviations of p from $\overline{p}$ on the control surface. $p = \overline{p}$ can be assumed.

$\left\langle \left(p - \overline{p}\right) \nabla X_i \right\rangle$ — Force due to deviations of p from $\overline{p}$ at the fluid interface – contact force

- **Multipressure formulation removes ill-posedness**

Contact force needs to be closed

- **It obeys Newton's third law as a contact force should.**
- **It is not dissipative force**
  - Distinction from "frictional" momentum exchange (drag force)
- **Due to these distinct features, change in unresolved kinetic energy (UKE) can be used for closing this term, leading to the functional form of the virtual mass term.**
  - Derived by J. D. Ramshaw (unpublished)

$$\left\langle \left(p-\overline{p}\right)\nabla X_i \right\rangle = C_{vm}\left(\frac{D_j\mathbf{u}_j}{Dt}-\frac{D_i\mathbf{u}_i}{Dt}\right)$$

- **Virtual mass force and the coefficient are "turbulence" quantities**

How do we close the virtual mass coefficient?

- **Since we know the functional form of virtual mass term, it is now the matter of determining the coefficient.**
  - Traditionally virtual mass coefficients in general two-phase flow regime have been obtained by various techniques, resulting in significant differences in details.
  - They nonetheless produce qualitative or semi-quantitative results.
- **DNS?**
- **More detailed theory**
- **Can we close them using experimental data for mixing?**
  - RT and RM with variable acceleration history
  - Approach developed by R. Rauenzahn (LA-UR-06-1522)

Closing virtual mass coefficient for mixing

- **Select an ODE model that well matches experimental data.**
  - Variable acceleration history
  - Impulsive acceleration mimics RM instability.
  - Can be viewed as representation of experimental data in an ODE form
  - J. D. Ramshaw's model (Phys. Rev. E **58**, 5834 (1998)) selected.
- **Transform the multi-phase model equations into an ODE form.**
  - Incompressible two fluids
  - Assumed volume fraction profile across the mix layer
  - Mixing (interpenetration) velocity profile obtained, leading to time evolution of mix layer (bubble height) thickness.
- **Then compare to the ODE and determine the virtual mass coefficient.**

$$\left\langle \left(p-\overline{p}\right)\nabla X_i \right\rangle = \alpha_i \alpha_j \left[\frac{\left(\rho_i+\rho_j\right)\lambda}{\pi\left(1+r\right)|h|} - \frac{\rho_i\rho_j}{\rho}\right]\left(\frac{D_j \mathbf{u}_j}{Dt} - \frac{D_i \mathbf{u}_i}{Dt}\right)$$

Frictional drag

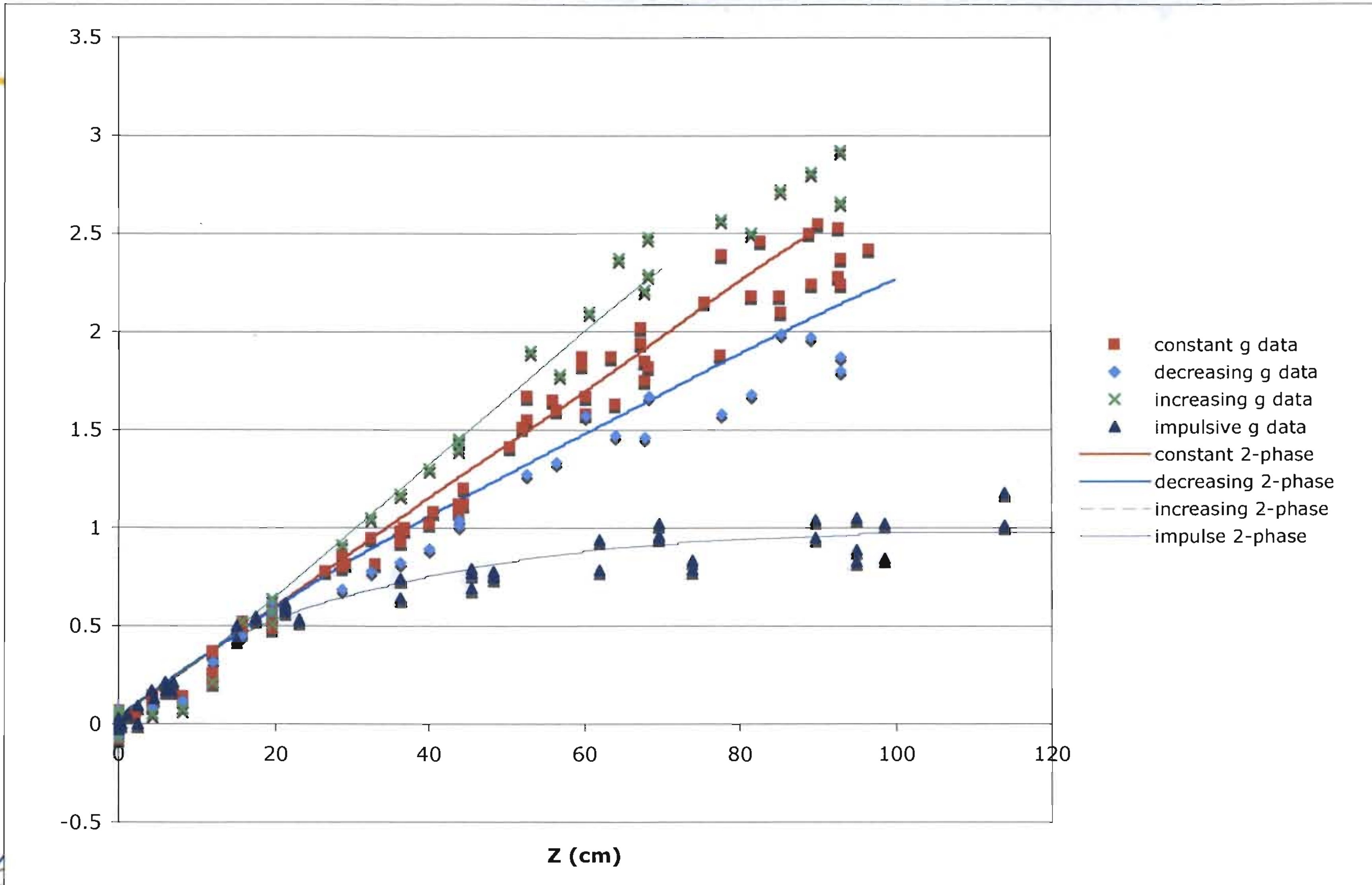
- **Approach used in obtaining the virtual mass coefficient also yields the drag coefficient, with results**

$$\mathbf{F}_{ij} = \alpha_i \alpha_j C_D \frac{(\rho_i + \rho_j)\left|\mathbf{u}_j - \mathbf{u}_i\right|}{\mu(1+r)\left|\mathbf{L}_{ij}\right|}(\mathbf{u}_j - \mathbf{u}_i)$$

$$\frac{\partial \mathbf{L}_{ij}}{\partial t} + \mathbf{u}_v \cdot \nabla \mathbf{L}_{ij} = \mathbf{u}_j - \mathbf{u}_i$$

- **Global nature of length scale (bubble height) does not fit well with multi-dimensional mixing simulations.**
- **Bell-Plesset effect on length scale**

Multi-fluid model comparison with LEM data



Strength effects

- S_i in $\nabla \cdot (\alpha_i \mathbf{S}_i)$ is replaced by the deviatoric stress τ_i
- Damage and failure automatically included.

$$\alpha_i \rho_i \left(\frac{\partial \mathbf{u}_i}{\partial t} + \mathbf{u}_i \cdot \nabla \mathbf{u}_i \right) = -\nabla\left[\alpha_i \left(p_i - p\right)\right] - \alpha_i \nabla p + \nabla \cdot \left(\alpha_i \tau_i\right) + \nabla \cdot \left(\alpha_i \mathbf{R}_i\right)$$
$$+ \sum_j \alpha_i \alpha_j \left[\frac{\left(\rho_i + \rho_j\right)\lambda}{\pi\left(1+r\right)\left|h\right|} - \frac{\rho_i \rho_j}{\rho} \right] \left(\frac{D_j \mathbf{u}_j}{Dt} - \frac{D_i \mathbf{u}_i}{Dt} \right)$$
$$+ \sum_j \mathbf{F}_{ij} + \mathbf{T}_i + \alpha_i \rho_i \mathbf{g}$$

- **Stress represented at mesh resolution level**
  - Strength effects included in simulations resolving surface irregularities.
- **How about simulations using coarse mesh?**

Subzonal strength effects

- **We close T_i (subzonal stress term) with existing ODE model (A. R. Piriz, et. al., Phys Rev E 80, 046305 (2009)), using a similar approach for closing the virtual mass coefficient.**
  - Although the functional form for contact force T_i with strength not derived, we can close the whole term.
  - Only magnitude of the term obtained. Direction is added by velocity differences

$$\mathbf{T}_i = \begin{cases} 2\alpha_i \alpha_j k G_s \dfrac{\mathbf{u}_j - \mathbf{u}_i}{\left|\mathbf{u}_j - \mathbf{u}_i\right|} & \text{if } h \le h_p \\ \xi \alpha_i \alpha_j \dfrac{Y_s}{\sqrt{3}h} \dfrac{\mathbf{u}_j - \mathbf{u}_i}{\left|\mathbf{u}_j - \mathbf{u}_i\right|} & \text{if } h > h_p \end{cases}$$

$$\text{where } h_p = \frac{\pi \xi Y_s}{\sqrt{3}\lambda_0 G_s},\ Y_s = \max\left(Y_i, Y_j\right),\ G_s = \max\left(G_i, G_j\right)$$

- **When perturbation is resolved, this term is not necessary.**
  - This term does not vanish gracefully as computation resolution increases.
  - Double counting.

All ingredients exist

$$\alpha_i\rho_i\left(\frac{\partial \mathbf{u}_i}{\partial t}+\mathbf{u}_i\cdot\nabla\mathbf{u}_i\right)=-\nabla\left[\alpha_i\left(p_i-p\right)\right]-\alpha_i\nabla p+\nabla\cdot\left(\alpha_i\tau_i\right)+\nabla\cdot\left(\alpha_i\mathbf{R}_i\right)$$

$$+\sum_j\alpha_i\alpha_j\left[\frac{\left(\rho_i+\rho_j\right)\lambda}{\pi\left(1+r\right)\left|h\right|}-\frac{\rho_i\rho_j}{\rho}\right]\left(\frac{D_j\mathbf{u}_j}{Dt}-\frac{D_i\mathbf{u}_i}{Dt}\right)$$

$$+\sum_j\alpha_i\alpha_j C_D\frac{\left(\rho_i+\rho_j\right)\left|\mathbf{u}_j-\mathbf{u}_i\right|}{\mu\left(1+r\right)L}\left(\mathbf{u}_j-\mathbf{u}_i\right)+\mathbf{T}_i+\alpha_i\rho_i\mathbf{g}$$

- **Virtual mass force and subzonal strength effects are consistent in linear growth regime.**
  - In nonlinear growth regime, strength effects disappear.
- **Reynolds stress currently ignored**
  - Double counting?
- **Pressure nonequilibrium**
  - Volume fraction evolution model required (C. H. Chang and J. D. Ramshaw, Phys. Rev. E **77**, 066305 (2008).)

Current status and further improvements

- Implementation currently under way
- Reynolds stress ignored
- Possible double counting of strength effects not resolved
- Ideal plasticity assumed
  - Damage
  - Failure
- Length scale model needs improvements
- Bell-Plesset effect not included
- A model transitioning from multiphase to multicomponent form has been developed.