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Investigation of Mixing Law Efficacy for Gaseous Hydrodynamic Simulations

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Overview

Introduction

- Gaseous Shock Tube Simulations
  - N_2 & SF_6/He Mixture
  - 1:1 & 1:3 SF_6/He (Mixture Ratios)
- Mixing EOS
  - Ideal, Amagat, Dalton
  - BKW, JCZ3, EXP6
- Post-Shock Properties
  - Shock Speed
  - Shock Pressure
  - Shock Temperature
- Model Form Error
  - **Missing non-equilibrium physics!**

History

Liquid Nitrogen

Zubarev & Telegin (1962); Ross & Ree (1980)

Solid Carbon Dioxide

Ross & Ree (1980)

Gaseous Argon

Davidson, et. al. (1998); Davidson & Henson (1996) — noted discrepancies between ideal predictions and experiments

Helium & Sulfur Hexafluoride

Wayne, et. al. (2019)

Equations of State

Ideal Gas

- EOS defines the relationship between the state variables
- Gases are often described by thee properties (P, T, & ν)
- Knowledge of any two properties yields the entire state

$$P\nu = RT$$

- Combination of Boyle's, Charles', Avogadro's, & Gay-Lussac's Laws
- Only applicable at low pressures & high temperatures
- Compressibility factor, z, accounts for non-ideal behaviour

$$P\nu = zRT$$

Amagat & Dalton

- Non-reacting gas mixtures behave ideal
- Assumption of which property is constant
- Dalton's Law of additive pressures

$$P_m = \sum_i^k P_i(T_m, V_m)$$

- Amagat's Law of additive volumes

$$V_m = \sum_i^k V_i(T_m, P_m)$$

BKW

- Becker-Kistiakowsky-Wilson EOS
- Used extensively to calculate detonation properties
- SNL BKW: $\alpha = 0.5, \beta = 0.298, \kappa = 10.5,$ & $\theta = 6620$

$$\frac{PV}{RT} = 1 + Xe^{\beta X}, \qquad X = \frac{\kappa \sum_i n_i k_i}{V(T+\theta)^\alpha}$$

JCZ3

- Jacobs-Cowperthwaite-Zwisler (JCZ) EOS
- E_o: Volume potential of face-centered cube lattice
- f: factor based on Helmholtz free energy
- Constant $\eta = 13$

$$P = \frac{G(V, T, \varphi)nRT}{V} + P_0(V, \varphi), \qquad G = 1 - \frac{V}{f}\left(\frac{\partial f}{\partial V}\right)_T, \qquad P_0 = -\frac{\mathrm{d}E_o}{\mathrm{d}V}$$

$$\varphi(r) = \varepsilon\left[\left(\frac{6}{\eta - 6}\right)\exp\left[\eta(1 - \frac{r}{r^*})\right] - \left(\frac{\eta}{\eta - 6}\right)\left(\frac{r^*}{r}\right)^6\right]$$

EXP6

- Similar formulation to JCZ3
- Contains several mixture rules
- Non-constant η

$$\eta = \frac{\sum_{i,j} x_i x_j \eta_{ij} \varepsilon_{ij} r_{ij}^3}{\varepsilon_m r_m^3}$$

Software

DAKOTA

- Design optimization, parameter estimation, uncertainty quantification, and sensitivity analysis framework
- Multidimensional parameter study capability
- Wraps around arbitrary software
- Developed by SNL

Tiger

- Thermodynamic equilibrium code
- Generates custom, tabular EOS
- Developed by SRI
- Updated & maintained by SNL

CTH & BCAT

- CTH:
  - Multidimensional, multi-material, large deformation, strong shock, solid mechanics code
  - Tabular EOS input capability
  - Domains: 1DL, 1DC, 1DR, 2DC, 2DR, 3DR
  - Lagrangian distortion step & Eulerian remap step
  - Developed at SNL
- BCAT:
  - CTH distribution package
  - Develops and tests EOS models
  - Converts Tiger EOS to SESAME format

Methodology

Amagat & Dalton Mixing

- Pure He & SF_6 tabular EOS generated by Tiger
- Mixed EOS created via summation
- Tiger utilizes specific variables

$$\omega = \frac{\Omega}{m}, \qquad m_i = M_i n_i$$

- Tiger normalizes number of moles

$$m_i = M_i x_i, \qquad x_i = \frac{n_i}{n_m}$$

- Mass fraction weighting

$$w_i = \frac{m_i}{m_m}$$

- Amagat Formulation

$$T_m = T_i, \qquad \nu_m = \sum_i w_i \nu_i, \qquad P_m = P_i, \qquad e_m = \sum_i w_i e_i, \qquad s_m = \sum_i w_i s_i$$

- Dalton Formulation
  - Note mass fraction weighting of specific volume

$$T_m = T_i, \qquad \nu_m = w_i \nu_i, \qquad P_m = \sum_i P_i, \qquad e_m = \sum_i w_i e_i, \qquad s_m = \sum_i w_i s_i$$

  - Prescribed specific volume range must be scaled

$$\nu_j = \nu_i \frac{m_i}{m_j}$$

Experimental Setup

- Driver:
  - 1.22 m long cylindrical tube, 7.62 cm ID
  - 0.75 m long rectangular tube, 7.62 cm inside square cross-section
- Driven:
  - Rectangular tube, 7.62 cm inside square cross-section

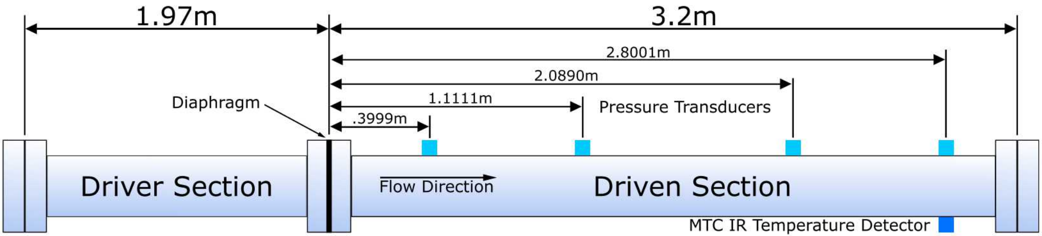


Figure: Notional Depiction of UNM Shock Tube

- Driver filled with Nitrogen: three initial pressures
- He/SF_6 mixture: three initial pressures
- Two molar concentrations

Table: Variable Experimental Parameters

P_{N_2} [kPa]	P_{He/SF_6} [kPa]	x_{He}
1006	39.3	50%
1145	78.6	75%
1282	118	

Mesh & Boundary Conditions

- Physical shock tube not modeled
- Unable to model cylindrical gaseous volume in 3D rectangular domain
  - Length scaled to maintain cross-sectional area & volume

$$V_{rect} = 4r^2 l_{rect}, \qquad V_{cyl} = \pi r^2 l_{cyl}, \qquad \Rightarrow \qquad l_{rect} = \frac{\pi}{4} l_{cyl}$$

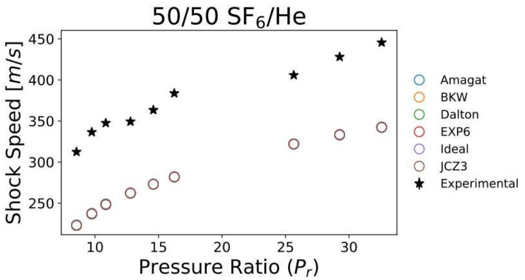
- No polyester diaphragm
- Reflective boundary conditions

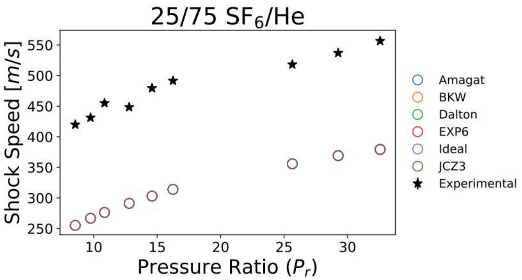
Simulation Procedure

- DAKOTA parametrizes 108 simulations in parallel.
- FOR every simulation, Python performs the following:
  1. Generate the TIGER input deck and execute TIGER to create the tabular EOS(s).
  2. IF Amagat or Dalton: Manually create mixed EOS.
  3. Generate BCAT input deck and execute BCAT to convert EOS to binary SESAME format.
  4. Generate CTH input deck and execute CTH to initialize the shock tube simulation.
  5. Calculate scalar quantities of interest.
- DAKOTA tabulates the QOI in a text file against initial parameters.

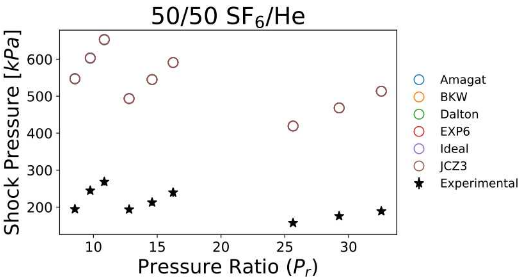
Results

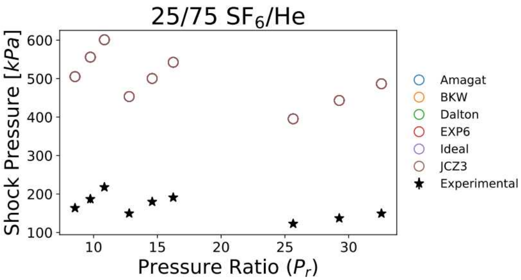
Shock Speed


50/50 SF_6/He
Shock Speed [m/s]
450
400
350
300
250
10
15
20
25
30
Pressure Ratio (P_r)
Amagat
BKW
Dalton
EXP6
Ideal
JCZ3
Experimental

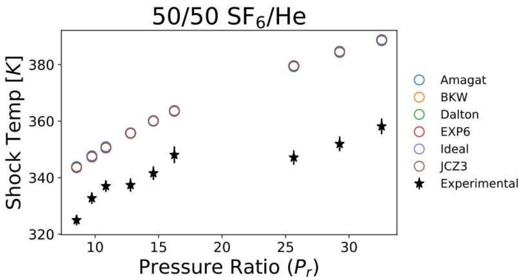

25/75 SF_6/He
Shock Speed [m/s]
550
500
450
400
350
300
250
10
15
20
25
30
Pressure Ratio (P_r)
Amagat
BKW
Dalton
EXP6
Ideal
JCZ3
Experimental

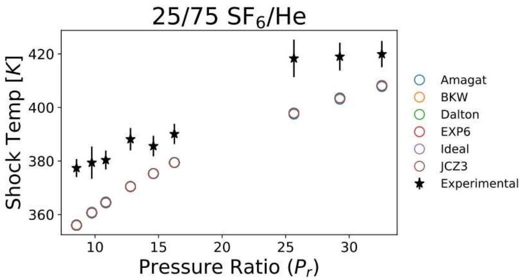
Shock Pressure





Shock Temperature





Summary

- Large discrepancies despite weak shock
- Similar results obtained from literature
- Discrepancy is too prominent — van der Waals eqs. unable to solely account
- Amagat & Dalton lack necessary physics to capture non-equilibrium shock effects

Questions?