

REAL-GAS EQUATIONS OF STATE FOR THE GASFLOW CFD CODE

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ABSTRACT

GASFLOW is a finite-volume computer code that solves the time-dependent, two-phase homogeneous equilibrium model, compressible Navier-Stokes equations for multiple gas species with turbulence. The fluid-dynamics algorithm is coupled with conjugate heat and mass transfer models to represent walls, floors, ceilings, and other internal structures to describe complex geometries, such as those found in nuclear containments and facilities. Recent applications involve simulations of cryogenic hydrogen tanks at elevated pressures. These applications, which often have thermodynamic conditions near the critical point, require more accurate real-gas equations of state (EOS) and transport properties than the standard ideal gas EOS and classical kinetic-theory transport properties. The standard for real-gas modeling is provided by the National Institute for Standards and Technology (NIST) in Boulder, Colorado. We have implemented Leachman's NIST hydrogen EOS as well as two simpler models: (1) a modified van der Waals EOS and (2) a modified Nobel-Abel EOS. Testing and verifying the real-gas EOS implementations is difficult, but most important to provide confidence in the new EOS model developments. A "numerically exact benchmark" problem has been especially developed to address these concerns. This report describes the rigorous implementation of the generalized real-gas EOS into the GASFLOW CFD code, as well as the specific implementation of respective real-gas models; it also includes a logical testing procedure based upon a numerically exact benchmark problem. An example of GASFLOW simulations is presented for an ideal cryocompressed hydrogen tank.

1.0 INTRODUCTION

The purpose of this report is to formulate the numerical procedure to implement generalized real-gas equations of state for the GASFLOW [1] semi-implicit-ALE CFD Code.

2.0 SIMPLIFIED GASFLOW EQUATION SET

For this discussion, a simplified GASFLOW Equation set is employed with the following assumptions: 1. Single fluid specie, 2. No phase change, 3. No heat and/or mass transfer, and 4. No chemical reactions to the following set of equations:

2.1 Volume Equation

$$\frac{\partial}{\partial t} V = V \nabla \cdot \mathbf{u} \quad (1)$$

2.2 Mixture Mass Equation

$$\frac{\partial}{\partial t} \rho = -\nabla \cdot (\rho \mathbf{u}) \quad (2)$$

2.3 Mixture Momentum Equations

$$\frac{\partial}{\partial t}(\rho \mathbf{u}) = -\nabla \cdot (\rho \mathbf{u} \mathbf{u}) - \nabla p + \nabla \cdot \boldsymbol{\tau} + \rho \mathbf{g} \quad (3)$$

2.4 Mixture Internal Energy Equation

$$\frac{\partial}{\partial t}(\rho I) = -\nabla \cdot (\rho \mathbf{u} I) - p \nabla \cdot \mathbf{u} - \nabla \cdot \mathbf{q} \quad (4)$$

2.5 General Thermodynamic Equation of State

$$P = P(\rho, T) = Z(\rho, T) \rho \frac{R}{M} T \quad (5)$$

2.6 General Caloric Equation of State

$$I = I(\rho, T) \quad (6)$$

3.0. THE ICE'D-ALE NUMERICAL METHODOLOGY

One can integrate the above equation set over regular finite volumes using a classical staggered-mesh with fluid scalars occupying control volume centroids, while velocities are located at control volume surfaces. This method is time-split into three distinct phases: A. An explicit Lagrangian “physics” phase; B. An implicit Lagrangian pressure propagation phase; and C. An explicit rezone or convection phase.

3.1 Phase A: Explicit Lagrangian Phase

All time advanced variables, with superscript “ A ”, can be determined from the beginning of the time cycle values denoted “ n ”.

3.1.1 Volume Equation

$$\frac{V^A - V^n}{\Delta t} = V^n \nabla \cdot \mathbf{u}^n \quad (7)$$

3.1.2 Mixture Mass Equation

$$\frac{(\rho V)^A - (\rho V)^n}{\Delta t} = 0 \quad (8)$$

3.1.3 Mixture Momentum Equations

$$\frac{(\rho V \mathbf{u})_m^A - (\rho V \mathbf{u})_m^n}{\Delta t} = -V_m^n \nabla p^n + V_m^n \nabla \cdot \boldsymbol{\tau}_m^n + \rho_m^n V_m^n \mathbf{g} \quad (9)$$

3.1.4 Mixture Internal Energy Equation

$$\frac{(\rho VI)^A - (\rho VI)^n}{\Delta t} = -V^n p^n \nabla \cdot \mathbf{u}^n - V^n \nabla \cdot \mathbf{q}^n \quad (10)$$

3.1.5 General Thermodynamic Equation of State

$$p(\rho^A, T^A) = Z(\rho^A, T^A) \rho^A \frac{R}{M} T^A \quad (11)$$

3.1.6 General Caloric Equation of State

$$I^A = I(\rho^A, T^A) \quad (12)$$

3.2 Phase B: Implicit Lagrangian Pressure Iteration Phase

3.2.1 Volume Equation

$$\frac{V^B - V^A}{\Delta t} = V^n \nabla \cdot [(\mathbf{u})^B - (\mathbf{u})^n] \quad (13)$$

3.2.2 Mixture Mass Equation

$$\frac{(\rho V)^B - (\rho V)^A}{\Delta t} = 0 \quad (14)$$

3.2.3 Mixture Momentum Equations

$$\frac{(\rho V \mathbf{u})_m^B - (\rho V \mathbf{u})_m^A}{\Delta t} = -V_m^n \nabla (p^B - p^n) \quad (15)$$

3.2.4 Mixture Internal Energy Equation

$$\frac{(\rho VI)^B - (\rho VI)^A}{\Delta t} = -V^n p^n \nabla \cdot (\mathbf{u}^B - \mathbf{u}^n) \quad (16)$$

3.2.5 The General Thermodynamic Equation of State

$$p(\rho^B, T^B) = Z(\rho^B, T^B) \rho^B \frac{R}{M} T^B \quad (17)$$

3.2.6 The General Caloric Equation of State

$$I^B = I(\rho^B, T^B) \quad (18)$$

Equations (13-18) can be combined into a single Poisson type expression. If equation (14) is considered, one can rewrite (16) as follows

$$\frac{(\rho V)^A}{\Delta t} (I^B - I^A) = \frac{(\rho V)^A}{\Delta t} \Delta I = -V^n p^n \nabla \cdot [\mathbf{u}^B - \mathbf{u}^n]. \quad (19)$$

With the aid of (14), the total differential of the caloric EOS (6) reads

$$\Delta I = \left(\frac{\partial I}{\partial \rho} \right)_T \Delta \rho + \left(\frac{\partial I}{\partial T} \right)_\rho \Delta T = - \left(\frac{\partial I}{\partial \rho} \right)_T \left(\frac{\rho}{V} \right) \Delta V + C_v \Delta T. \quad (20)$$

Multiplying the Thermodynamic EOS (5) by V gives

$$pV = \left(\rho V \frac{R}{M} \right) \cdot Z(\rho, T) \cdot T \quad (21)$$

before taking the total differential

$$\Delta(pV) = \left(\rho V \frac{R}{M} \right) \cdot (Z \cdot \Delta T + T \cdot \Delta Z), \quad (22)$$

where

$$\Delta Z = \left(\frac{\partial Z}{\partial \rho} \right)_T \Delta \rho + \left(\frac{\partial Z}{\partial T} \right)_\rho \Delta T = - \left(\frac{\partial Z}{\partial \rho} \right)_T \left(\frac{\rho}{V} \right) \Delta V + \left(\frac{\partial Z}{\partial T} \right)_\rho \Delta T. \quad (23)$$

Substituting (23) into (22) yields

$$\Delta(pV) = \left(\rho V \frac{R}{M} \right) \left\{ \left[Z + T \left(\frac{\partial Z}{\partial T} \right)_\rho \right] \Delta T - T \left(\frac{\partial Z}{\partial \rho} \right)_T \left(\frac{\rho}{V} \right) \Delta V \right\}. \quad (24)$$

Using (21) and solving for ΔT gives

$$\Delta T = \frac{\left[\Delta(pV) + \left(\frac{pV}{Z} \right) \left(\frac{\partial Z}{\partial \rho} \right)_T \left(\frac{\rho}{V} \right) \Delta V \right]}{\left[\left(\frac{pV}{T} \right) + \left(\frac{pV}{Z} \right) \left(\frac{\partial Z}{\partial T} \right)_\rho \right]} = \frac{\left[\Delta(pV) + C_1^A \Delta V \right]}{C_2^A}, \quad (25)$$

where the constants C_1^A and C_2^A are evaluated at split time-level ‘‘A’’, and are given by

$$C_1^A = \left[\left(\frac{pV}{Z} \right) \left(\frac{\partial Z}{\partial \rho} \right)_T \left(\frac{\rho}{V} \right) \right]^A = \left[\left(\frac{R}{M} T \frac{(\rho V)^2}{V^2} \right) \left(\frac{\partial Z}{\partial \rho} \right)_T \right]^A \quad (26)$$

and

$$C_2^A = \left[\left(\frac{pV}{T} \right) + \left(\frac{pV}{Z} \right) \left(\frac{\partial Z}{\partial T} \right)_\rho \right]^A = \left[\left(\frac{pV}{T} \right) + \left(\rho V \right) \frac{R}{M} T \left(\frac{\partial Z}{\partial T} \right)_\rho \right]^A. \quad (27)$$

Substituting (25) into (20) gives

$$\Delta I = \left[C_v \frac{C_1^A}{C_2^A} - \left(\frac{\partial I}{\partial \rho} \right)_T \left(\frac{\rho}{V} \right) \right] \Delta V + \frac{C_v}{C_2^A} \Delta(pV) \quad (28)$$

before substituting this result (28) into (19) to produce

$$(\rho V)^A \left\{ \left[C_v \frac{C_1^A}{C_2^A} - \left(\frac{\partial I}{\partial \rho} \right)_T \left(\frac{\rho}{V} \right) \right] \Delta V + \frac{C_v}{C_2^A} \Delta(pV) \right\} = -\Delta t V^n p^n \nabla \cdot [\mathbf{u}^B - \mathbf{u}^n], \quad (29)$$

or when (13) is introduced on the right hand side of (29)

$$(\rho V)^A \left\{ \left[C_v \frac{C_1^A}{C_2^A} - \left(\frac{\partial I}{\partial \rho} \right)_T \left(\frac{\rho}{V} \right) \right] \Delta V + \frac{C_v}{C_2^A} \Delta(pV) \right\} = -p^n \Delta V, \quad (30)$$

and then collecting terms gives

$$(\rho V)^A \frac{C_v}{C_2^A} \Delta(pV) = - \left[p^n + (\rho V)^A \left[C_v \frac{C_1^A}{C_2^A} - \left(\frac{\partial I}{\partial \rho} \right)_T \left(\frac{\rho}{V} \right) \right] \right] \Delta V. \quad (31)$$

Introducing additional constants (from the evaluation at split time-level ‘‘A’’ again) gives

$$C_3^A \Delta(pV) = -C_4^A \Delta V, \quad (32)$$

where

$$C_3^A = \left[(\rho V) \frac{C_v}{C_2^A} \right]^A \quad (33)$$

and

$$C_4^A = p^n + (\rho V)^A \left[C_v \frac{C_1^A}{C_2^A} - \left(\frac{\partial I}{\partial \rho} \right)_T \left(\frac{\rho}{V} \right) \right]^A. \quad (34)$$

Adding and subtracting $p^A V^B$ on the left hand side of (32) gives

$$(p^B V^B - p^A V^B + p^A V^B - p^A V^A) = -\frac{C_4^A}{C_3^A} (V^B - V^A) \quad (35)$$

or

$$\Delta p = (p^B - p^A) = - \left(p^A + \frac{C_4^A}{C_3^A} \right) \frac{(V^B - V^A)}{V^B}. \quad (36)$$

This equation can be linearized by rearranging $\frac{(V^B - V^A)}{V^B}$, and then applying a binomial series to obtain

$$\frac{(V^B - V^A)}{V^B} \cong \frac{(V^B - V^A)}{V^A}, \quad (37)$$

provided $\frac{(V^B - V^A)}{V^A} \ll 1$, to produce

$$(p^B - p^A) = -\left(p^A + \frac{C_4^A}{C_3^A}\right) \frac{(V^B - V^A)}{V^A}. \quad (38)$$

Consider the volume conservation equation (13), where by adding and subtracting \mathbf{u}^A inside the divergence operator, one obtains

$$V^B - V^A = \Delta t V^n \nabla \cdot [\mathbf{u}^B - \mathbf{u}^A + \mathbf{u}^A - \mathbf{u}^n] = \Delta t V^n \nabla \cdot [\mathbf{u}^B - \mathbf{u}^A] + \Delta t V^n \nabla \cdot [\mathbf{u}^A - \mathbf{u}^n]. \quad (39)$$

Equation (39) can be introduced into (38) to give

$$(p^B - p^A) = -\left(p^A + \frac{C_4^A}{C_3^A}\right) \frac{\Delta t V^n \nabla \cdot [\mathbf{u}^B - \mathbf{u}^A]}{V^A} - \left(p^A + \frac{C_4^A}{C_3^A}\right) \frac{(\Delta t V^n \nabla \cdot [\mathbf{u}^A - \mathbf{u}^n])}{V^A}. \quad (40)$$

The momentum conservation equation (15) with the help of the mass conservation equation (14) and $\delta p = p^B - p^n$, can be written as

$$\mathbf{u}^B - \mathbf{u}^A = \frac{\Delta t}{(\rho_m V_m)^A} V_m^n [-\nabla(p^B - p^n)] = -\Delta t \frac{V_m^n}{(\rho_m V_m)^A} \nabla \delta p, \quad (41)$$

which when substituted into (40), yields

$$\Delta t^2 \nabla \cdot \left[\frac{V_m^n}{(\rho_m V_m)^A} \nabla \delta p \right] - \frac{V^A}{V^n} \frac{(\delta p)}{\left(p^A + \frac{C_4^A}{C_3^A}\right)} = \frac{V^A}{V^n} \frac{(p^n - p^A)}{\left(p^A + \frac{C_4^A}{C_3^A}\right)} + \Delta t \nabla \cdot [\mathbf{u}^A - \mathbf{u}^n], \quad (42)$$

where

$$\frac{C_4^A}{C_3^A} = \frac{p^n + (\rho V)^A \left[c_v(T, \rho) \frac{\left[\rho^2 \left(\frac{R}{M} \right)_T \left(\frac{\partial Z}{\partial \rho} \right)_T \right]}{\left[\left(\frac{pV}{T} \right) + (\rho V) \left(\frac{R}{M} \right)_T \left(\frac{\partial Z}{\partial T} \right)_\rho \right]} - \left(\frac{\partial I}{\partial \rho} \right)_T \left(\frac{\rho}{V} \right) \right]^A}{\left[(\rho V) \frac{c_v(T, \rho)}{\left[\left(\frac{pV}{T} \right) + (\rho V) \left(\frac{R}{M} \right)_T \left(\frac{\partial Z}{\partial T} \right)_\rho \right]} \right]^A}. \quad (43)$$

This equation is 2nd order and linear in δp . After solving this Poisson type pressure change Equation (42), one can then back substitute δp into (41) to determine \mathbf{u}^B , $p^B = p^n + \delta p$, V^B from (13), ρ^B from (14), T^B from inverting (17), and I^B from either (16) or (18).

3.3 Phase C: Explicit Eulerian (Convection) Phase

All advanced time variables with superscript “B” have been determined from the previous phase. One can now complete the time cycle to values “n+1” by performing the convection phase.

3.3.1 Volume Equation

$$V^{n+1} = V^n \quad (44)$$

3.3.2 Mixture Mass Equation

$$\frac{(\rho V)^{n+1} - (\rho V)^B}{\Delta t} = -V^n \nabla \cdot (\rho \mathbf{u})^B \quad (45)$$

3.3.3 Mixture Momentum Equations

$$\frac{(\rho_m V_m \mathbf{u})^{n+1} - (\rho_m V_m \mathbf{u})^B}{\Delta t} = -V_m^n \nabla \cdot (\rho \mathbf{u} \mathbf{u})^B \quad (46)$$

3.3.4 Mixture Internal Energy Equation

$$\frac{(\rho V I)^{n+1} - (\rho V I)^B}{\Delta t} = -V^n \nabla \cdot (\rho \mathbf{u} I)^B \quad (47)$$

3.3.5 The General Thermodynamic Equation of State

$$p(\rho^{n+1}, T^{n+1}) = Z(\rho^{n+1}, T^{n+1}) \rho^{n+1} \frac{R}{M} T^{n+1} \quad (48)$$

3.3.6 The General Caloric Equation of State

$$I^{n+1} = I(\rho^{n+1}, T^{n+1}) \quad (49)$$

3.4 The summation of the complete computational cycle yields the following:

3.4.1 Mixture Mass Equation

$$\frac{(\rho V)^{n+1} - (\rho V)^n}{\Delta t} = -V^n \nabla \cdot (\rho \mathbf{u})^B \quad (50)$$

3.4.2 Mixture Momentum Equations

$$\frac{(\rho_m V_m \mathbf{u})^{n+1} - (\rho_m V_m \mathbf{u})^n}{\Delta t} = -V_m^n \nabla \cdot (\rho \mathbf{u} \mathbf{u})^B - V_m^n \nabla p^B + V_m^n \nabla \cdot \boldsymbol{\tau}_m^n + \rho_m^n V_m^n \mathbf{g} \quad (51)$$

3.4.3 Mixture Internal Energy Equation

$$\frac{(\rho V I)^{n+1} - (\rho V I)^n}{\Delta t} = -V^n \nabla \cdot (\rho \mathbf{u} I)^B - V^n p^n \nabla \cdot \mathbf{u}^B - V^n \nabla \cdot \mathbf{q}^n \quad (52)$$

4.0 SOME EXAMPLE EQUATIONS OF STATE FOR THE ABOVE ANALYSIS

4.1 Ideal Gas: $p(\rho, T) = \rho \frac{R}{M} T$ and $I(T) = I_{ig}(T)$

$$\left(\frac{\partial Z}{\partial \rho} \right)_T = 0, \left(\frac{\partial Z}{\partial T} \right)_\rho = 0, \text{ and } \left(\frac{\partial I}{\partial \rho} \right)_T = 0$$

4.2 Modified Nobel-Abel: $p(\rho, T) = \frac{\rho \frac{R}{M} T}{c - b\rho}$ and $I(T) = I_{ig}(T)$

$$\left(\frac{\partial Z}{\partial \rho} \right)_T = \frac{b}{(c - b\rho)^2}, \left(\frac{\partial Z}{\partial T} \right)_\rho = 0, \text{ and } \left(\frac{\partial I}{\partial \rho} \right)_T = 0$$

The coefficients “ b ” and “ c ”, in the above Modified Nobel-Abel EOS, for the 2 hydrogen thermodynamic states:

(245 K, 2.5 MPa, 2.43277 kg/m³), and (35 K, 2.5 MPa, 49.66182 kg/m³).

can be found as:

$b = -0.040026142924481$ and $c = 0.886493850623252$.

The motivation that these 2 particular thermodynamic states were selected for fitting the 2 coefficients is demonstrated in Section 5 below.

4.3 Modified van der Waals: $p(\rho, T) = \frac{\rho \frac{R}{M} T}{c - b\rho} - a\rho^2$ and $I(\rho, T) = I_{ig}(T) - a\rho$

$$\left(\frac{\partial Z}{\partial \rho} \right)_T = \frac{b}{(c - b\rho)^2} - \frac{M}{R} \frac{a}{T}, \left(\frac{\partial Z}{\partial T} \right)_\rho = a \left(\frac{\rho}{T^2} \right) \left(\frac{M}{R} \right), \text{ and } \left(\frac{\partial I}{\partial \rho} \right)_T = -a$$

The coefficients “ a ”, “ b ” and “ c ” in the above Modified van der Waals EOS for the 3 hydrogen thermodynamic states:

(245 K, 2.5 MPa, 2.43277 kg/m³), (35 K, 2.5 MPa, 49.66182 kg/m³), and (61.5 K, 25 MPa, 64.2 kg/m³).

can be found as:

$a = 4.70470053582692E+3$, $b = 9.81499353729889E-3$, and $c = 0.996969112920896$.

The reason these 3 thermodynamic states were selected for fitting the 3 coefficients is demonstrated in Section 6 below.

4.4 Leachman’s NIST: Modern equations of state [2,3] are often formulated using the Helmholtz energy as the fundamental property with independent variables of temperature and density,

$$\alpha(T, \rho) = \alpha^0(T, \rho) + \alpha^r(T, \rho), \tag{53}$$

where α is the Helmholtz energy, $\alpha^0(T, \rho)$ is the ideal gas contribution to the Helmholtz energy, and $\alpha^r(T, \rho)$ is the residual Helmholtz energy, which corresponds to the influence of intermolecular forces. Thermodynamics properties can be calculated as derivatives of the Helmholtz energy. For example, the pressure is

$$p = \rho^2 \left(\frac{\partial \alpha}{\partial p} \right)_T \quad (54)$$

In practical applications, the functional form is explicit in the dimensionless Helmholtz energy, α , using independent variables of dimensionless density and temperature. The form of this equation is

$$\frac{\alpha(T, \rho)}{RT} = \alpha(\tau, \delta) = \alpha^0(\tau, \delta) + \alpha^r(\tau, \delta), \quad (55)$$

where $\tau = T_c/T$, the inverse reduced temperature and $\delta = \rho/\rho_c$, the reduced density.

The ideal gas Helmholtz energy is represented in the computational convenient parameterized form

$$\alpha^0(\tau, \delta) = \ln \delta + 1.5 \ln \tau + a_1 + a_2 \tau + \sum_{k=3}^N a_k \ln [1 - \exp(b_k \tau)], \quad (56)$$

and the residual contribution to the Helmholtz free energy takes the form

$$\alpha^r(\tau, \delta) = \sum_{i=1}^l N_i \delta^{d_i} \tau^{t_i} + \sum_{i=l+1}^m N_i \delta^{d_i} \tau^{t_i} \exp(-\delta^{p_i}) + \sum_{i=m+1}^n N_i \delta^{d_i} \tau^{t_i} \exp \left[+\varphi_i (\delta - D_i)^2 + \beta_i (\tau - \gamma_i)^2 \right], \quad (57)$$

where the parameters and coefficients for parahydrogen and normal hydrogen are given by Leachman^{1,2}.

The advantages of this new explicit formulation in the Helmholtz free energy become apparent in the calculation of the various properties:

$$\text{Pressure: } p(T, \rho) = \rho RT \left[1 + \delta \left(\frac{\partial \alpha^r}{\partial \delta} \right)_\tau \right], \quad (58)$$

$$\text{Compressibility factor: } Z(T, \rho) = \frac{p}{\rho RT} = 1 + \delta \left(\frac{\partial \alpha^r}{\partial \delta} \right)_\tau, \quad (59)$$

$$\text{Internal energy: } u(T, \rho) = RT \tau \left[\left(\frac{\partial \alpha^0}{\partial \tau} \right)_\delta + \left(\frac{\partial \alpha^r}{\partial \tau} \right)_\delta \right], \text{ and} \quad (60)$$

$$\text{Isochoric heat capacity: } c_v(T, \rho) = -R \tau^2 \left[\left(\frac{\partial^2 \alpha^0}{\partial \tau^2} \right)_\delta + \left(\frac{\partial^2 \alpha^r}{\partial \tau^2} \right)_\delta \right]. \quad (61)$$

Some derivatives required for the GASFLOW real gas formulation Equations (42) and (43) are:

$$\left(\frac{\partial Z}{\partial \rho}\right)_T = \delta \left(\frac{\partial^2 \alpha^r}{\partial \delta^2}\right)_\tau \left(\frac{\partial \delta}{\partial \rho}\right) + \left(\frac{\partial \alpha^r}{\partial \delta}\right)_\tau \left(\frac{\partial \delta}{\partial \rho}\right) = \frac{1}{\rho_c} \left[\delta \left(\frac{\partial^2 \alpha^r}{\partial \delta^2}\right)_\tau + \left(\frac{\partial \alpha^r}{\partial \delta}\right)_\tau \right]$$

$$\left(\frac{\partial Z}{\partial T}\right)_\rho = \delta \left(\frac{\partial^2 \alpha^r}{\partial \delta \partial \tau}\right) \left(\frac{\partial \tau}{\partial T}\right) = -\frac{\delta \tau}{T} \left(\frac{\partial^2 \alpha^r}{\partial \delta \partial \tau}\right) = -\frac{\rho}{\rho_c} \frac{T_c}{T^2} \left(\frac{\partial^2 \alpha^r}{\partial \delta \partial \tau}\right)$$

$$\left(\frac{\partial I}{\partial \rho}\right)_T = \frac{R}{M} T_c \left[\left(\frac{\partial^2 \alpha^0}{\partial \tau \partial \delta}\right) \left(\frac{\partial \delta}{\partial \rho}\right) + \left(\frac{\partial^2 \alpha^r}{\partial \tau \partial \delta}\right) \left(\frac{\partial \delta}{\partial \rho}\right) \right] = -\frac{R}{M} \frac{T^2}{\rho} \left(\frac{\partial Z}{\partial T}\right)_\rho = \frac{R}{M} \frac{T_c}{\rho_c} \left(\frac{\partial^2 \alpha^r}{\partial \delta \partial \tau}\right)$$

5.0 A NUMERICALLY EXACT BENCHMARK PROBLEM FOR MODEL VERIFICATION

The implementation of real gas equations of state in CFD codes is a difficult task. For this reason, testing and verifying such implementation is important to provide the code developers and users confidence that the required development and coding has been correctly accomplished. This section provides a numerically exact benchmark problem to help developers and users gain that confidence.

One can describe a time-dependent, one-dimensional, filling problem. A schematic drawing of the problem is shown in Fig. 1. A short tube is filled with hydrogen at 2.5 MPa and 245 K. Initially there is a constant velocity from the bottom toward to top at a slow velocity of 1 cm/s exiting out the top at the same velocity. Magically, cold hydrogen at 35 K and 25 MPa is introduced into the bottom of the tube with the same inflowing velocity of 1 cm/s. The problem is to compute the cold hydrogen pushing the warmer hydrogen out the tube top in a constant pressure process. Clearly, the cold hydrogen will completely fill the tube in 10 s, so the problem time is specified greater than 1 s, but less than 10 s.

5.1 Analysis using a Real Gas Equation of State

An exact numerical solution can be found for the above stated benchmark problem from the following hyperbolic “system”; conservation of mass and energy plus the caloric and thermodynamic equations of state constraints (in further discussions, these equations are referred simply as the *system*):

$$\frac{\partial}{\partial t}(\rho) + \frac{\partial}{\partial x}(\rho u) = 0 \quad (62)$$

$$\frac{\partial}{\partial t}(\rho h) + \frac{\partial}{\partial x}(\rho h u) = 0 \quad (63)$$

$$h(T, \rho) = RT \left\{ \tau \left[\left(\frac{\partial \alpha^0}{\partial \tau}\right)_\delta + \left(\frac{\partial \alpha^r}{\partial \tau}\right)_\delta \right] + \delta \left(\frac{\partial \alpha^r}{\partial \delta}\right)_\tau + 1 \right\} \quad (64)$$

$$p(T, \rho) = \rho RT \left[1 + \delta \left(\frac{\partial \alpha^r}{\partial \delta}\right)_\tau \right] \quad (65)$$

Note that Equation (65) can be substituted into Equation (64) resulting in 3 Equations in 3 unknowns (ρ , T , and u), which must be iteratively solved until the above *system* is satisfied.

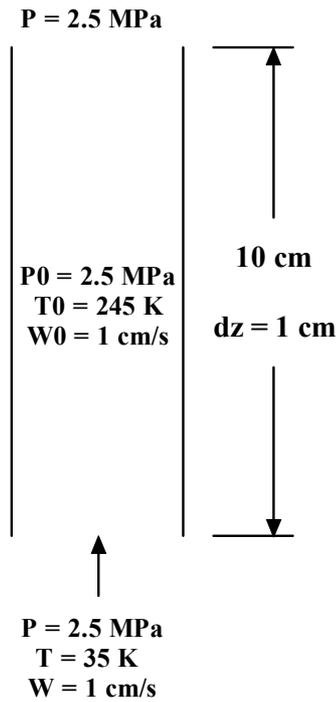


Figure 1. A Schematic Drawing for the time-dependent, one-dimensional Benchmark Filling Problem.

5.2 Exact Numerical and GASFLOW Solutions for the Benchmark

Figure 2 and Figure 3 show, respectively a comparison of the temperature and density profiles found from the exact numerical solution of the *system* and the GASFLOW solution for the inviscid gas dynamics equations (Euler Equations) using 1st order upwind differencing, 2nd order Lax-Wendroff, and 2nd order TVD MC (van Leer [4]). These three convective schemes are implemented in GASFLOW, and this is the reason the analysis carried forward focuses around these schemes. We are satisfied with these results; and consequently, believe that the real-gas EOS has been correctly implemented into the GASFLOW code.

6.0. EXAMPLE OF AN IDEAL (NO STRUCTURAL HEAT TRANSFER) CRYOCOMPRESSED TANK FILLING SIMULATION

A cryocompressed hydrogen tank, shown schematically in Figure 4, can be filled with 35 K hydrogen from initial to final conditions, see Table 1: Stage 0. Decompressing the tank from the initial conditions to 2.5 MPa, Stage 1. Cooling the tank by filling 35 K hydrogen with constant pressure of 2.5 MPa, and Stage 2. Charging the tank with 35 K hydrogen to 25 MPa. The thermodynamic paths are presented in Figure 5. Table 2 gives the GASFLOW computed process times for two filling rates 20 and 100 kg/hr, respectively. The simulations exactly follow the thermodynamic paths in Figure 5.

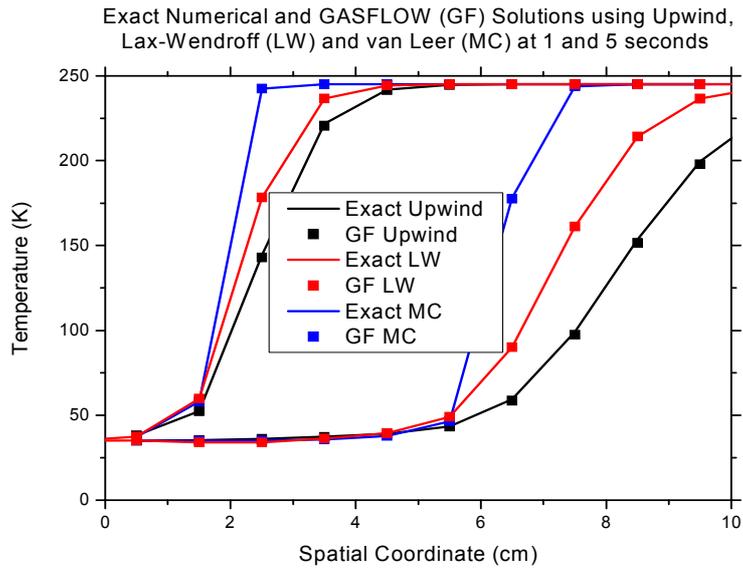


Figure 2. Comparison of the Exact Numerical (*System*) and GASFLOW Solutions computed on a uniform 1 cm mesh showing the Temperature Distributions for Upwind differencing, Lax-Wendroff differencing and TVD MC (van Leer) limiter.

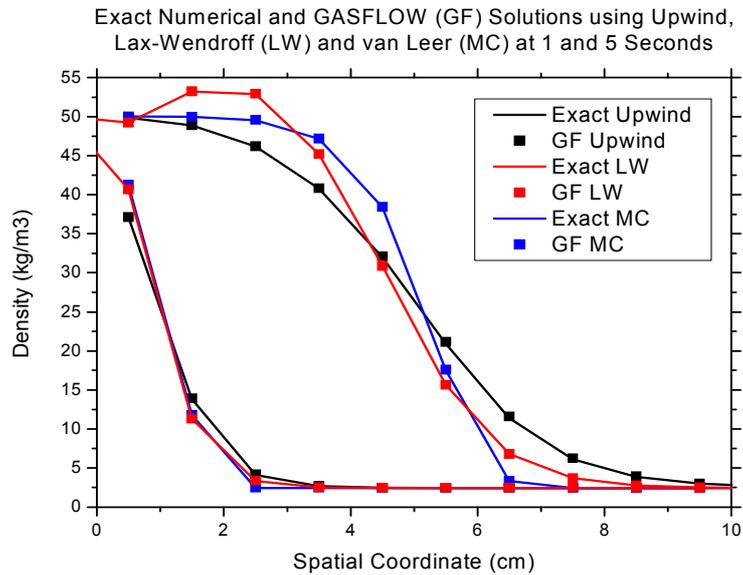


Figure 3. Comparison of the Exact Numerical (*System*) and GASFLOW Solutions computed on a uniform 1 cm mesh showing the Density Distributions for Upwind differencing, Lax-Wendroff differencing and TVD MC (van Leer) limiter.

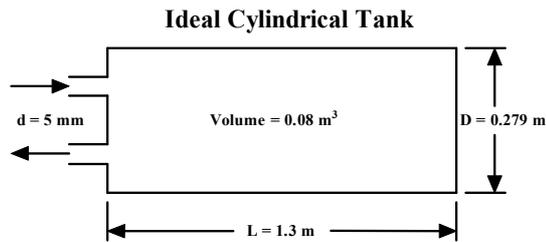


Figure 4. Simple Schematic Model of a Cryocompressed Hydrogen Tank.

Table 1. Initial and Final Conditions for an Ideal Filling a Cryocompressed Tank with Hydrogen

Conditions	Pressure (MPa)	Temperature (K)	Density (kg/m ³)
Initial	5	300	3.9
Final	25	61.5	64.2

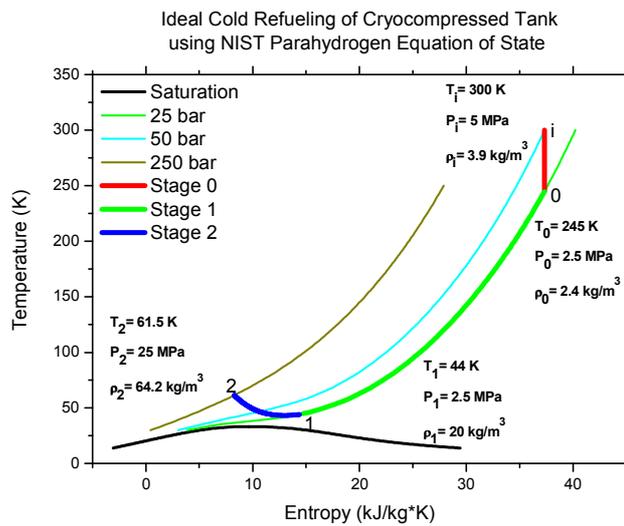


Figure 5. The Thermodynamics of Filling a Cryocompressed Tank with Hydrogen.

Table 2. Ideal GASFLOW Results for two Cryocompressed Tank Filling Rates

Filling Rates (kg/hr)	Stage 0 Time (s)	Stage 1 Time (s)	Stage 2 Time (s)	Total Time (s)
20	5	270	630	905
100	5	55	125	185

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