A Generic Non-Miscible Liquid-Gas Medium Model in Modelica with Analysis of Incompressibility Assumptions

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Abstract

Motivated by the representation of draining or leak scenarios in industrial processes, this paper introduces a generic two-phase non-miscible liquid-gas medium model. The model represents two distinct substances with independent thermodynamic states and enables transient simulations involving phase-separated liquid and gas domains. It is designed to remain compatible with the Modelica.Media and Modelica.Fluid interfaces. In developing this model, we analyze how specific assumptions about liquid compressibility — such as the dependency of enthalpy and density on pressure — affect the structure of the resulting balance equations through detailed mathematical analysis. We examine different incompressibility approaches and their implications for the formulation of conservation equations. This article focuses on a comprehensive theoretical analysis of the model formulation, highlighting the trade-offs involved and providing insights into selecting appropriate liquid models for dynamic simulations involving non-miscible flows.

Keywords: Liquid-Gas Medium, Draining and Leak Scenario, Incompressibility, Numerical Robustness, Small Modular Reactor

1 Introduction

The Modelica language (Modelica Association 2017) provides a powerful, equation-based environment for the dynamic simulation of complex physical systems, particularly thermal-hydraulic networks (Fritzson 2014). Libraries such as the Modelica Standard Library [MSL] `Modelica.Fluid`, Buildings (Wetter et al. 2014), AixLib (Müller et al. 2016), and ThermoFluidStream (Zimmer, Meißner, and Weber 2022) offer rich sets of components governed by the underlying thermodynamic properties encapsulated in replaceable `Medium` models via the `Modelica.Media` interface.

This framework is well suited for the analysis of advanced concepts, including new generation nuclear reactors: Small Nuclear Reactors (SMRs). Molten Salt Reactors (MSRs), for instance, present demanding simulation requirements due to their unique characteristics and operational scenarios (Serp et al. 2014). Applying Modelica to specific MSR transients, like draining or leak management, has highlighted challenges in modeling systems that transition from a fully liquid (molten salt) state to a fully gaseous (inert gas) state via non-miscible phase interactions.

Most components (pipes, pumps, volumes, etc.) within the `Modelica.Fluid` library — and related libraries based on the same design philosophy — are capable of simulating single-phase liquid or gas flows, as well as equilibrium two-phase flows (e.g., liquid-vapor equilibrium) (Casella and Leva 2024). These components typically rely on media definitions based on a single thermodynamic state and often assume local phase equilibrium when modeling two-phase flows. However, several applications —such as the simulation of draining scenarios or gas ingress— require the ability to model liquid and gas phases as coexisting but strictly non-miscible, without assuming thermodynamic equilibrium. In SMR safety studies, for instance, transient configurations may include the loss or recovery of coolant, resulting in domains where both gas and liquid are present but governed by distinct physical laws. Beyond the nuclear domain, similar configurations are also found in other industrial processes involving large storage tanks, fluid circuit maintenance, or safety-related depressurization events.

To address these needs, we propose a new generic Modelica medium that models two non-miscible substances while maintaining compatibility with the existing ecosystem of components. The proposed `BisubLiqGas` medium allows independent specification of compressibility assumptions for each substance. In particular, it enables the user to represent incompressible or weakly compressible liquids while preserving full thermodynamic modeling of the gas (as perfect gas). The model is designed for seamless integration with `Modelica.Fluid` components, allowing mixed-phase simulations across pipes, tanks, or valves. This allows simulation of systems that transition seamlessly between fully liquid, fully gaseous, or mixed states using standard components.

Creating such a medium, however, necessitates careful consideration of how the individual phases are modeled, particularly the liquid. Molten salts, like many liquids, are often approximated as incompressible for simplicity. Yet, incompressibility ($\rho = f(T)$ only) can lead to different modeling variants regarding the pressure dependency of thermodynamic properties like internal energy u and enthalpy h. For example, defining enthalpy solely as $h(T)$ versus allowing an implicit pressure dependency leads to different system behavior, as detailed in Section 3. The choice of how to model liquid incompressibility and its thermodynamic consequences therefore becomes a critical aspect, impacting the robustness and efficiency of simulations involving such media.

The main contributions are thus twofold: (1) the presentation of a generic, standard-component-compatible `Medium` model for non-miscible liquid-gas systems, and (2) a detailed mathematical analysis of the trade-offs associated with different representations of liquid incompressibility within this context. Through rigorous derivation of conservation equations, we analyze the structural consequences of these modeling choices and their implications for equation complexity and physical accuracy. Our focus is on the theoretical and structural aspects of the medium formulation, providing a foundation for future implementation and performance studies.

The paper is structured as follows:

- Section 2 introduces a non-miscible two-substance `Medium` model (`BisubLiqGas`), detailing its formulation, assumptions, and general capabilities and limitations, applicable to various liquid-gas pairs.
- Section 3 delves into the core analysis of this paper: the modeling of liquid incompressibility. It discusses different incompressibility approaches and presents a comparative study, focusing on how different incompressibility assumptions impact the structure of the equations generated for a typical test case.

2 Non-miscible liquid-gas medium model

To represent the thermohydraulic behavior of the molten salt/cover gas mixture in scenarios such as draining or leak management, where the liquid and gas phases remain macroscopically separated, a specific medium model has been developed. This model, named `BisubLiqGas`, is designed to capture the essential properties of the mixture while maintaining manageable complexity for dynamic system simulation.

2.1 Medium Components

The `BisubLiqGas` medium is a binary mixture composed of two substances: one is a liquid (indexed L in formulas) and the second a gas (indexed G). While the specific substances used for illustration stem from the original MSR context (Molten Salt and Helium), the model's structure allows for generic application, as detailed in Section 2.5.

- **Liquid substance (Molten Salt)**: The specific model used is from the TRANSFORM library `TRANSFORM.Media.Fluids.NaClKClMgCl2.LinearNaClKClMgCl2_30_20_50_pT` (Greenwood et al. 2023). This choice implies modeling the ternary salt as a fluid whose density is a linear function of temperature T and pressure p, and whose specific heat capacity at constant pressure Cp_L is assumed constant:

$$\rho_L(p,T) = \rho_{L,ref}\left[1-\beta\cdot(T-T_{ref})+\kappa\cdot(p-p_{ref})\right] \tag{1}$$

where $\rho_{L,ref}$, T_{ref}, and p_{ref} are the reference density, temperature, and pressure, respectively, and β and κ are the constant isobaric expansion and isothermal compressibility coefficients. The values for these constants and the transport properties (dynamic viscosity η_L, thermal conductivity λ_L) are derived from correlations or experimental data specific to this molten salt (Greenwood et al. 2023).

- **Gas substance (Helium)**: The standard MSL model `Media.IdealGases.SingleGases.He` is used. This implies that Helium is treated as an ideal gas:

$$p\cdot V = n\cdot R\cdot T \quad \Leftrightarrow \quad p = \rho\cdot R_s\cdot T \tag{2}$$

where $R_s = R/MM_G$ is the specific gas constant for Helium. Furthermore, its specific heat capacity at constant pressure Cp_G is assumed constant and equal to $\frac{5}{2}R_s$, the theoretical value for a monoatomic ideal gas:

$$Cp_G = \frac{5}{2}\cdot R_s = \text{constant} \tag{3}$$

2.2 Fundamental Assumptions of the Mixture Model

The `BisubLiqGas` model relies on the following key assumptions for the mixture:

- **Non-miscibility**: The liquid (salt) and gas (helium) phases are considered completely immiscible. No dissolution of the gas into the liquid or vice versa is modeled. The interface between the phases is assumed to be sharp within components using this medium.
- **Absence of Phase Change**: No evaporation, condensation, solidification, or fusion is considered. The salt remains liquid, and the Helium remains gaseous throughout the simulated operating range.
- **Local Thermal Equilibrium**: Within an elementary control volume, both phases are assumed to be at the same temperature T.
- **Local Mechanical Equilibrium**: Within an elementary control volume, both phases are assumed to be at the same pressure p. (Note: Hydrostatic pressure differences can exist at the component level).

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- **Ideal Thermodynamic Mixing**: The specific enthalpy and internal energy of the mixture are calculated as the mass-fraction weighted average of the respective pure phase properties, implying no heat of mixing.

2.3 Implementation and State Variables

The model is implemented by inheriting from `MSL.Media.Interfaces.PartialMedium`. The chosen independent thermodynamic state variables are pressure p, temperature T, and mass fractions X (`ThermoStates.pTX` option). The liquid substance is considered as X_1 and gas as X_2. The model provides the standard set of functions required by the `PartialMedium` interface to compute thermodynamic and transport properties from various input variable combinations (e.g., `density(setState_phX(...))`, `temperature(setState_psX(...))`). The implementation ensures that calls to component property functions use the appropriate pure substance state derived from the mixture's p and T.

2.4 Mixing Rules

The thermodynamic and transport properties of the mixture are calculated from the properties of the pure components *Liq* and *Gas* (evaluated at the mixture's pressure p and temperature T) using the following mixing rules:

- **Density** (ρ): Derived from the additivity of volumes ($V = V_L + V_G$) and the definition of mass fractions ($m_i = X_i m$), using the linear equation of state for the liquid (1) and the ideal gas law (2) for the gas:

$$\rho(p,T,X) = \frac{m_L + m_G}{V_L + V_G} = \frac{\rho_L(p,T)}{X_L + X_G \frac{\rho_L(p,T) R_s T}{p}} \tag{4}$$

- **Specific Enthalpy** (h): Calculated by mass weighting, consistent with the ideal mixing assumption:

$$h(p,T,X) = X_L \cdot h_L(p,T) + X_G \cdot h_G(p,T) \tag{5}$$

  where h_L is given by integrating Cp_L and accounting for the pressure dependency (from the linear model), and h_G is given by $Cp_G(T - T_0)$, with a consistent reference temperature T_0 (here $0\,°\mathrm{C}$).

- **Specific Internal Energy** (u): Derived from enthalpy and density:

$$u(p,T,X) = h(p,T,X) - \frac{p}{\rho(p,T,X)} \tag{6}$$

  This is equivalent to the mass-weighted average $u = X_L \cdot u_L + X_G \cdot u_G$.

- **Other Properties (Approximation)**: To simplify the model, other mixture properties Y_{mix} (dynamic viscosity η, thermal conductivity λ, specific entropy s, specific heat capacities Cp and c_v, isentropic exponent γ, speed of sound a) are approximated by a simple mass weighting of the pure phase properties:

$$Y_{mix}(p,T,X) \approx X_L \cdot Y_L(p,T) + X_G \cdot Y_G(p,T) \tag{7}$$

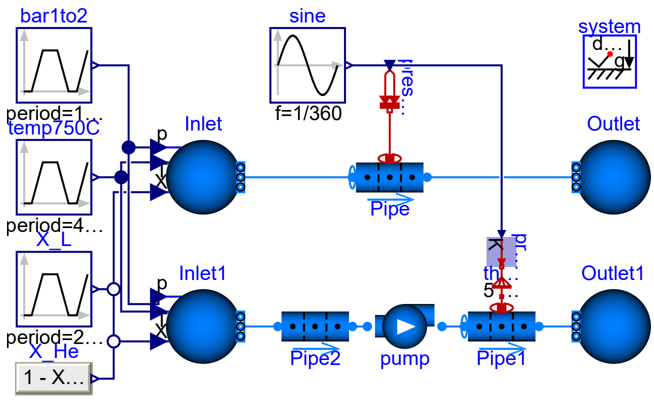

Figure 1. Unit test schematic using the `BisubLiqGas` model with a `DynamicPipe`.

2.5 Model Capabilities and Limitations

The `BisubLiqGas` medium model provides a framework for simulating systems containing non-miscible liquid-gas mixtures using standard Modelica fluid components.

2.5.1 Current Status and Validation

The model demonstrates functionality in several unit tests, such as simulating transient inlet conditions for a `Modelica.Fluid.Pipes.DynamicPipe` component (an example setup is shown in Figure 1). However, achieving robust performance across the full range of standard fluid components and complex scenarios remains an area of ongoing work. Challenges can arise from component-specific assumptions incompatible with a two-substance medium or from the numerical properties of the medium representation itself. Investigating these aspects, particularly the different approaches to modeling liquid incompressibility as discussed in Section 3, is a key objective of this paper.

2.5.2 Compatibility and Genericity

While initially motivated by an MSR application (molten salt/helium), the `BisubLiqGas` model is structured for broader applicability. The choice of liquid and gas substances can be adapted by replacing the specific component models, provided they adhere to the required base interfaces:

- **Liquid Substance**: The medium model for the liquid phase shall extend `Media.Interfaces.PartialLinearFluid`
- **Gas Substance**: The medium model for the gas phase shall extend `Media.`

`IdealGases.Common.SingleGasNasa` (or provide a compatible interface). While the base `SingleGasNasa` models can handle temperature-dependent properties, the enthalpy calculation within the `BisubLiqGas` mixing rules (Eq. (5)) currently assumes a constant specific heat capacity Cp_G (e.g., $5/2R_s$ for Helium) for simplicity in the implementation of inverse functions like `setState_phX`. This simplification should be considered when selecting or adapting the gas model for high-accuracy simulations over wide temperature ranges. The C_p for monatomic ideal gas is $5R/2$ and the value for diatomic ideal gas is $7R/2$.

2.5.3 Inherent Limitations

The use of the `BisubLiqGas` model is subject to the following fundamental limitations stemming from its core assumptions and implementation choices:

- **Component Model Validity**: The overall model validity is restricted to the pressure and temperature ranges where the chosen gas model (e.g., ideal gas behavior for Helium) and the chosen liquid model (e.g., linear approximation for the specific salt) remain acceptable representations of the real substance properties.
- **Non-Miscibility Assumption**: The assumption of perfect non-miscibility must hold. The model does not account for any solubility of the gas in the liquid or vice versa.
- **No Phase Change**: The model cannot simulate scenarios involving phase transitions (boiling, condensation, solidification, melting). Both substances are assumed to remain in their initial liquid or gas state.
- **Mixing Rule Approximations**: The linear mass-weighting rule (Eq. (7)) used for transport properties (dynamic viscosity η, thermal conductivity λ) and several thermodynamic properties (specific entropy s, specific heat capacities c_p, c_v, isentropic exponent γ, speed of sound a) is a significant simplification for non-miscible mixtures. The accuracy impact, especially for η, λ, and a, depends heavily on the specific substances and flow regime, and must be carefully evaluated for the target application.
- **Local Equilibrium Assumption**: The assumptions of local thermal and mechanical equilibrium (uniform T and p for both phases within a control volume) may break down in very rapid transients or highly heterogeneous flows.

Despite these limitations, the `BisubLiqGas` model provides a practical basis for studying dynamic system-level scenarios involving non-miscible liquid-gas mixtures where macroscopic phase separation is dominant, such as draining transients or tank pressurization/depressurization, using standard Modelica components.

3 Liquid state management

In this section, we will focus solely on the liquid substance and more specifically on the treatment of thermodynamic relationships and the handling of incompressibility aspects.

A terminological clarification is necessary because the use of the term incompressible is sometimes ambiguous. In this article, we will use the following terms with precise meanings:

- **Incompressible**: refers to a fluid whose density is constant (invariant with respect to all state variables)
- **Zero compressibility**: refers to a fluid whose isothermal compressibility is zero (or negligible), meaning that the density, which normally depends on temperature and pressure, does not vary with pressure but may vary with temperature

Let us recall that isothermal compressibility is defined by:

$$\chi_T = -\frac{1}{V} \cdot \left(\frac{\partial V}{\partial p}\right)_T = \frac{1}{\rho} \cdot \left(\frac{\partial \rho}{\partial p}\right)_T \tag{8}$$

In a single-species, single-phase fluid, the usual state variables are pressure, density, and temperature. Mass and energy balances provide equations for 2 of the 3 state variables. The closure equation is given by the fluid properties, particularly its equation of state.

The problem with liquids is that the equation of state often results in very small variations of density with pressure (low isothermal compressibility). This can cause numerical issues because pressure is often used as an explicit variable in state functions where density appears more in balance equations. We name an explicit variable one that is used as input to state functions. In this article, the following approaches will be defined and compared:

- Incompressible approach
- Semi-incompressible approach where density remains constant except in the mass conservation equation and in the buoyancy term of momentum conservation, where it is only a function of temperature. This is the counterpart of the Boussinesq approximation for system-scale calculations.
- Zero compressibility approach (density independent of pressure but dependent on temperature)
- Zero compressibility approach combined with the elimination of pressure force work in the internal energy and enthalpy relationships used in the energy balance

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The objective is to study the impact of deviations from rigorous thermodynamic relationships in favor of potentially better numerical performance.

3.1 Mathematical descriptions of the liquid state equations

First, let's establish the differentials of thermodynamic relations as functions of pressure and temperature.

3.1.1 Density

$$d\rho = \left(\frac{\partial \rho}{\partial p}\right)_T \cdot dp + \left(\frac{\partial \rho}{\partial T}\right)_p \cdot dT \tag{9}$$

By introducing the definition of isothermal compressibility χ_T (Eq. 8) and the definition of the isobaric thermal expansion coefficient α (Eq. 10), we obtain the differential of density (Eq. 11):

$$\alpha = \frac{1}{V} \cdot \left(\frac{\partial V}{\partial T}\right)_p = -\frac{1}{\rho} \cdot \left(\frac{\partial \rho}{\partial T}\right)_p \tag{10}$$

α can be expressed using the density ρ instead of the volume V by applying the variable change $V = m/\rho$. The mass contained in the volume being constant during the transformation.

$$d\rho = \rho \cdot (\chi_T \cdot dp - \alpha \cdot dT) \tag{11}$$

3.1.2 Internal Energy

Specific internal energy, often used for isochoric transformations and expressed as a function of temperature and density, can also be expressed as a function of pressure and temperature.

The Gibbs identity is given by:

$$dU = T \cdot dS - p \cdot dV \tag{12}$$

We assume that entropy S and volume V are functions of temperature T and pressure p :

$$S = S(T, p), \quad V = V(T, p) \tag{13}$$

By injecting the differentials of the expressions of S and V into the identity of dU (Eq. 12), we obtain:

$$\left(\frac{\partial U}{\partial T}\right)_p = T \cdot \left(\frac{\partial S}{\partial T}\right)_p - p \cdot \left(\frac{\partial V}{\partial T}\right)_p \tag{14}$$

$$\left(\frac{\partial U}{\partial p}\right)_T = T \cdot \left(\frac{\partial S}{\partial p}\right)_T - p \cdot \left(\frac{\partial V}{\partial p}\right)_T \tag{15}$$

Simplifying the partial derivative with respect to temperature by introducing the heat capacity coefficient (at constant pressure (Eq. 16)):

$$C_p = T \cdot \left(\frac{\partial S}{\partial T}\right)_p \tag{16}$$

the partial derivative of the internal energy can be expressed as function of α (Eq. 10) and C_p (Eq. 16):

$$\left(\frac{\partial U}{\partial T}\right)_p = C_p - p \cdot V \cdot \alpha \tag{17}$$

Continuing with the partial derivative with respect to pressure. To simplify the expression, we use one of Maxwell's relations.

$$\left(\frac{\partial S}{\partial p}\right)_T = -\left(\frac{\partial V}{\partial T}\right)_p \tag{18}$$

By injecting this relation into the expression of $\left(\frac{\partial U}{\partial p}\right)_T$, we obtain:

$$\left(\frac{\partial U}{\partial p}\right)_T = -T \cdot \left(\frac{\partial V}{\partial T}\right)_p - p \cdot \left(\frac{\partial V}{\partial p}\right)_T \tag{19}$$

We can now simplify this relation by introducing the isobaric thermal expansion coefficient α (Eq. 10) and the isothermal compressibility coefficient χ_T (Eq. 8).

$$\left(\frac{\partial U}{\partial p}\right)_T = -\alpha \cdot T \cdot V \ + \ p \cdot V \cdot \chi_T \tag{20}$$

Finally, let's express the differential of internal energy using only these coefficients.

$$dU = (C_p - \alpha \cdot p \cdot V) \cdot dT + (-\alpha \cdot T \cdot V + p \cdot V \cdot \chi_T) \cdot dp \tag{21}$$

This expression is general and applies to any real fluid as long as the volume can be expressed as a function of T and p. This equation remains valid when all extensive quantities are expressed per unit mass.

3.1.3 Enthalpy

$$dH = \left(\frac{\partial H}{\partial T}\right)_p \cdot dT + \left(\frac{\partial H}{\partial p}\right)_T \cdot dp \tag{22}$$

To determine the differential, let's combine the internal energy differential (Eq. 21) and a relation between enthalpy and internal energy (Eq. 23) and the differential of volume (Eq. **??**):

$$H = U + p \cdot V \tag{23}$$

$$dH = dU + p \cdot dV + V \cdot dp$$

When replacing dV by its differential (Eq. **??**) and simplifying by the compensating term, the differential of the enthalpy is obtained:

$$dH = C_p \cdot dT + V \cdot (1 - T \cdot \alpha) \cdot dp \tag{24}$$

This expression is the general differential form of specific enthalpy as a function of temperature and pressure, involving calorimetric and thermoelastic coefficients.

3.2 Mathematical descriptions of the studied approaches

3.2.1 Incompressible approach

Recall that in this approach, the density is constant and invariant with respect to all state variables ($\alpha = 0$ and $\chi_T = 0$):

The differentials of internal energy (Eq. 21) and enthalpy (Eq. 24) are then considerably simplified:

$$dU = C_p \cdot dT \tag{25}$$

$$dH = C_p \cdot dT + V \cdot dp \tag{26}$$

The problem with this approach comes from the impossibility of modeling natural circulation, density driven flows, because the driving force of the flow, induced by density variation, is zero. Therefore, we will introduce the semi-incompressible approach to tackle this problem.

3.2.2 Semi-incompressible approach

In this approach, the differentials of internal energy (25) and enthalpy (26) remain unchanged compared to the incompressible approach. Only the differential of density is modified. Actually this density relation is only used in the mass balance equation and in the buoyancy term of the momentum balance equation:

$$d\rho = -\rho \cdot \alpha \cdot dT \tag{27}$$

3.2.3 Zero compressibility approach

In this approach, the isothermal compressibility is zero ($\chi_T = 0$), which means that density is independent of pressure but can vary with temperature. From the differential of density (Eq. 11), we obtain:

$$d\rho = -\rho \cdot \alpha \cdot dT \tag{28}$$

The differentials of internal energy (Eq. 21) and enthalpy (Eq. 24) then become:

$$dU = (C_p - \alpha \cdot p \cdot V) \cdot dT \; - \; \alpha \cdot T \cdot V \cdot dp \tag{29}$$

$$dH = C_p \cdot dT + V \cdot (1 - \alpha \cdot T) \cdot dp \tag{30}$$

By noting that $\alpha \cdot p \cdot V \cdot dT = p \cdot dV$, we can find the classic form:

$$dH = dU \; + \; p \cdot dV \; + \; V \cdot dp \tag{31}$$

The zero compressibility approach is more realistic for liquids, where density variation with temperature is significant (allowing modeling of buoyancy effects), while variation with pressure is often negligible.

3.2.4 Neglected pressure work approach

In this approach, we maintain the zero compressibility assumption ($\chi_T = 0$), but we also assume that pressure work is negligible in the enthalpy equation, which means that enthalpy depends only on temperature:

$$dH = C_p \cdot dT \tag{32}$$

If we now calculate the differential of internal energy from the relationship between internal energy and enthalpy (Eq. 23), we obtain:

$$dU = C_p \cdot dT - p \cdot dV - V \cdot dp \tag{33}$$

With the zero compressibility assumption, we can express the differential of volume directly as a function of the differential of temperature which gives:

$$dU = (C_p - p \cdot V \cdot \alpha) \cdot dT \; - \; V \cdot dp \tag{34}$$

By comparing with the expression of dU obtained with the differential of internal energy assuming zero compressibility (Eq. 29), we can quantify the bias induced by this assumption of negligible pressure work. The bias is therefore:

$$\begin{aligned} \delta dU &= dU_{\delta W=0} - dU_{\chi_T=0} \\ &= -V \cdot dp - (-\alpha \cdot T \cdot V \cdot dp) \\ &= -V \cdot (1 - \alpha \cdot T) \cdot dp \end{aligned} \tag{35}$$

This simplified approach can be useful numerically, but it leads to a thermodynamic inconsistency that can affect the accuracy of the simulation, particularly in cases where pressure variations are significant.

3.3 Conservation equations

Let's establish the mass balance for a fixed volume of a single-species single-phase fluid.

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3.3.1 Conservation of mass

$$V \cdot \frac{\mathrm{d}\rho}{\mathrm{d}t} = \sum_{boundaries} \dot{m} \tag{36}$$

Since the mass flow rate is a function of pressure, it is preferable to choose pressure as one of the explicit variables. With the assumption of a single-phase fluid, it is preferable to take temperature as the second explicit variable.

The left term of the continuity equation (Eq. 36) expressed as a function of temperature and pressure derives using the differential of the density (Eq. 11):

The right term is a function of the mass flow rate at the boundaries of the volume. By simplifying the flow as non-inertial, the mass flow rate becomes exclusively a function of the pressure losses at the boundaries. The calculation of the pressure losses requires having the value of the density and temperature to calculate the transport properties.

$$\dot{m} = f(\Delta p, \rho, T) \tag{37}$$

According to the scheme used to compute the flow rate (upstream, centered, order 1, 2 etc), the indices of the density, temperature and pressure differ. However, the general form is preferred to study the non linear behavior. Please note that implicit forms can raised depending on the scheme used. For clarity sake, a simplified centered scheme can be used in this section.

Grouping the left and right terms, we obtain:

$$V \cdot \rho \cdot \left(\chi_T \cdot \frac{\mathrm{d}p}{\mathrm{d}t} - \alpha \cdot \frac{\mathrm{d}T}{\mathrm{d}t} \right) = \sum f(\Delta p, \rho, T) \tag{38}$$

Let's now apply the assumptions of the different approaches to this equation.

Incompressible approach: Since the density is constant, the derivatives of the density with respect to pressure and temperature are zero. The density is always used to calculate the pressure losses but is no longer a function of the explicit variables, so it is removed from the function "f". The equation (Eq. 38) becomes a simple algebraic equation.

$$0 = \sum f(\Delta p, T) \tag{39}$$

Semi-incompressible approach: Since the density is only a function of temperature, it can be removed from the function "f". The equation (Eq. 38) can be simplified to:

$$\frac{\mathrm{d}T}{\mathrm{d}t} = \frac{\sum f(\Delta p, T)}{-\rho \cdot V \cdot \alpha} \tag{40}$$

We can clearly see with this approach that:

- The mass conservation equation becomes an equation for the time derivative of temperature
- The equation is linear and the derivative is explicit (does not depend on itself or on another time derivative)

Zero compressibility approach: The expression for density is exactly the same as for the semi-incompressible approach. The conclusions are therefore the same.

Neglected pressure work approach: The expression for density is exactly the same as for the semi-incompressible approach. The conclusions are therefore the same.

3.3.2 Conservation of energy

Let's apply the same process to the energy balance.

$$V \cdot \frac{\mathrm{d}(\rho \cdot u)}{\mathrm{d}t} = \sum_{boundaries} \dot{H} + \sum_{boundaries} \dot{Q} \tag{41}$$

For the energy balance, we will neglect external thermal inputs ($\sum \dot{Q}$). They do not change the conclusions.

The gross enthalpy flow $\dot{H}$ is the product of the mass flow rate and the specific enthalpy. From (Eq. 37), the mass flow rate can be expressed from the explicit variables:

$$\dot{H} = \dot{m} \cdot h = \sum f(\Delta p, \rho, T) \cdot h \tag{42}$$

According to the scheme used to compute the flow rate (upstream, centered, order 1, 2 etc), the indices of the density, temperature, pressure and enthalpy differ. However, the general form is preferred to study the non linear behavior. Please note that implicit forms can raised depending on the scheme used. For clarity sake, a simplified centered scheme can be used in this section.

Using Eq. 41 with the partial derivatives form and the Eq. 37:

$$\frac{\mathrm{d}p}{\mathrm{d}t} \cdot \rho \cdot V \cdot \left[\frac{\partial u}{\partial p} + u \cdot \chi_T \right] + \frac{\mathrm{d}T}{\mathrm{d}t} \cdot \rho \cdot V \cdot \left[\frac{\partial u}{\partial T} - u \cdot \alpha \right] = \sum (f(\Delta p, \rho, T) \cdot h) \tag{43}$$

Incompressible approach: Since density is constant and specific internal energy depends only on temperature, many partial derivatives become zero. Equation (43) becomes:

$$\frac{\mathrm{d}T}{\mathrm{d}t} = \frac{\sum (f(\Delta p, T) \cdot h)}{\rho \cdot V \cdot c_p} \tag{44}$$

- The energy conservation equation becomes an equation for the time derivative of temperature

- The equation is linear and the derivative is explicit (does not depend on itself). However, the right-hand term is also a function of pressure via the specific enthalpy formula.

Semi-incompressible approach: Since density and specific internal energy depend only on temperature, many partial derivatives become zero. Equation (43) becomes:

$$\frac{\mathrm{d}T}{\mathrm{d}t} = \frac{\sum (f(\Delta p, T)\cdot h)}{\rho \cdot V \cdot (c_p - \alpha \cdot u)} \tag{45}$$

The conclusions are identical to the incompressible approach. The only difference comes from the term in the denominator, which is corrected for the expansion effect.

Zero compressibility approach: The energy conservation equation (43) becomes:

$$\frac{\mathrm{d}p}{\mathrm{d}t}\cdot V \cdot (-\alpha \cdot T) + \frac{\mathrm{d}T}{\mathrm{d}t}\cdot \rho \cdot V \cdot \left[\left(c_p - \frac{p\cdot\alpha}{\rho}\right) - u\cdot\alpha\right] = \sum (f(\Delta p, T)\cdot h) \tag{46}$$

- The equations are linear and the derivative is explicit (does not depend on itself).
- The resolution of pressure is no longer an algebraic system but becomes an ordinary differential equation.

Zero compressibility + neglected pressure work approach: Since density and enthalpy depend only on temperature, the energy conservation equation (43) becomes:

$$\frac{\mathrm{d}p}{\mathrm{d}t}\cdot V \cdot \rho \cdot \left[\frac{\partial u}{\partial p}\right] + \frac{\mathrm{d}T}{\mathrm{d}t}\cdot V \cdot \left[\rho \cdot \frac{\partial u}{\partial T} + u \cdot \frac{\partial \rho}{\partial T}\right] = \sum f_2(\Delta p, T) \tag{47}$$

Note that for the formulation of internal energy, we cannot use equation (21) but (34), which derives from enthalpy without the pressure force work term. Moreover, the function f can be replace by f2 since the specific enthalpy depends only on temperature:

$$\frac{\mathrm{d}p}{\mathrm{d}t}\cdot(-V) + \frac{\mathrm{d}T}{\mathrm{d}t}\cdot \rho \cdot V \cdot \left[c_p - \frac{p\cdot\alpha}{\rho} - u\cdot\alpha\right] = \sum f_2(\Delta p, T) \tag{48}$$

3.4 Applicability of `TableBased` medium on these approaches

In this section, we will explain why the pre-existing generic `TableBased` medium of the MSL are not perfectly suited to our needs. All the four approaches presented in previous section cannot be reproduced with this medium by tuning the following parameters:

- singleState
- enthalpyOfT

For reminder, the definition of the singleState parameter is given in the MSL package `Media.UsersGuide.MediumUsage.Constants` and is as follows:

> singleState = true, if u and d are not a function of pressure, and thus only a function of a single thermal variable (temperature or enthalpy) and of Xi for a multiple substance medium. Usually, this flag is true for incompressible media. It is used in a model to determine whether 1+nXi (singleState=true) or 2+nXi (singleState=false) initial conditions have to be provided for a volume element that contains mass and energy balance.

For a purely incompressible approach, we must therefore have $singleState = true$. However, looking more closely at the system of equations, we find that $singleState = true$ is not always the right condition for the mass density and specific internal energy to depend only on temperature.

If $enthalpyOfT = false$, the function for calculating specific enthalpy (h_pT) becomes:

$$h = h_0 + \int_{T_0}^{T} cp \cdot dT + \frac{p - p_{ref}}{\rho}\cdot(1 - \alpha \cdot T) \tag{49}$$

If the density is constant (incompressible total), this expression simplifies to:

$$h = h_0 + \int_{T_0}^{T} cp \cdot dT + \frac{p - p_{ref}}{\rho} \tag{50}$$

The function for calculating specific internal energy with $singleState = true$ becomes:

$$u = h - \frac{p_{ref}}{\rho} \tag{51}$$

By substituting the expression for specific enthalpy, we obtain:

$$\begin{aligned} u =& h_0 + \int_{T_0}^{T} cp \cdot dT + \frac{p - p_{ref}}{\rho} - \frac{p_{ref}}{\rho} \\ u =& h_0 + \int_{T_0}^{T} cp \cdot dT + \frac{p}{\rho} \end{aligned} \tag{52}$$

We can clearly see that the pressure is always present in the expression for specific internal energy. On the contrary, if $singleState = false$, the function for calculating specific internal energy becomes:

$$\begin{aligned} u =& h_0 + \int_{T_0}^{T} cp \cdot dT + \frac{p - p_{ref}}{\rho} - \frac{p}{\rho} \\ u =& h_0 + \int_{T_0}^{T} cp \cdot dT - \frac{p_{ref}}{\rho} \end{aligned} \tag{53}$$

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In this case, specific internal energy and mass density are well independent of pressure. **However, we have the opposite behavior compared to what the user expects**. Moreover, this can cause problems with initialization because with singleState = false, the pressure is initialized in the capacitive components but has no inertial term.

If now $enthalpyOfT = true$ and $singleState = true$, the function to calculate specific enthalpy (h_T) becomes:

$$h = h_0 + \int_{T_0}^{T} cp \cdot dT \tag{54}$$

and the specific internal energy (u_T) becomes:

$$u = h_0 + \int_{T_0}^{T} cp \cdot dT - \frac{p_{ref}}{\rho} \tag{55}$$

Since the mass density is constant, the expression is independent of pressure.

The **semi-incompressible approach** could be modeled with the TableBased medium in the MSL. It would require forcing the constant $DensityOfT = false$ even though the density is a function of temperature. Indeed, the constantis defined as $DensityOfT = size(tableDensity, 1) > 1$. The parameters would then be:

- singleState = false
- enthalpyOfT = false
- densityOfT = false

The approach of **zero compressibility** cannot be modellable with the TableBased medium in the MSL even with the following parameters:

- singleState = false
- enthalpyOfT = false
- densityOfT = true

Introducing the (49) in the expression $u = h - \frac{p}{\rho}$, it can be remarked that there is the missing following term, which is a correction term of the specific heat capacity (check (29)) in the specific internal energy expression:

$$\int_{T_0}^{T} -\alpha \cdot \frac{p}{\rho} \cdot dT$$

Similarly, the approach of **zero compressibility + neglected pressure work** cannot be modeled with the TableBased medium in the MSL for the same reason than for the zero compressibility approach.

Based on the analysis operated in this section, our further developments must concern the modeling of a own liquid medium for the bisubtance model rather than using an existing medium from the Modelica Standard Library (MSL) in order to:

- Build expertise in medium development
- Have total control over the approximations made
- The TableBased medium in the MSL rebuilds polynomials from data points. It does not allow defining arbitrary relationships between variables.

4 Comparison of approaches applied to a flow in a vertical pipe

Let us now attempt to quantify the differences between the approaches by applying them to a simple case: the flow in a vertical adiabatic pipe. In this article, we will focus exclusively on the theoretical study. A further study is ongoing and will contain the practical comparison using an equivalent Modelica model, compiled and executed with OpenModelica.

Suppose a perfectly adiabatic vertical pipe filled with an inert liquid fluid (no heat production). Let's start by assuming that the fluid is static. We can generalize later. The conservation of energy gives us an invariance of the sum of enthalpy and potential energy of gravity.

$$dH + m \cdot g \cdot dz = 0 \tag{56}$$

Replacing dH by its exact expression:

$$C_p \cdot dT + V \cdot (1 - T \cdot \alpha) \cdot dp + m \cdot g \cdot dz = 0 \tag{57}$$

We can express dp in terms of dz using the hydrostatic relation:

$$dp = -\rho \cdot g \cdot dz \tag{58}$$

The conclusions remain valid even when introducing a term for pressure loss: $dp = -\rho\ g\ dz\ -\ dp_{loss}$

$$C_p \cdot dT + V \cdot (1 - T \cdot \alpha) \cdot (-\rho \cdot g \cdot dz) + m \cdot g \cdot dz = 0 \tag{59}$$

By simplifying the terms that cancel out and dividing by the mass ($m = \rho\ V$), we obtain:

$$c_p \cdot dT + T \cdot \alpha \cdot g \cdot dz = 0 \tag{60}$$

We can therefore determine the temperature variation as a function of height variation:

$$\frac{dT}{dz} = \frac{-\alpha \cdot T \cdot g}{c_p} \tag{61}$$

NB: With a mass density that depends on temperature, a temperature change induces a change in mass density. By mass conservation, in steady state, this induces a change in flow rate, hence kinetic energy. The energy balance should therefore be written:

$$H + \frac{1}{2} \cdot m \cdot V^2 + m \cdot g \cdot (z - z_0) = \text{constant} \tag{62}$$

We choose to neglect the effects of kinetic energy for simplicity.

For a real transformation with fluid displacement, we make a change of variable to make the pressure loss term appear in the hydrostatic equation (58). In practice, a pressure loss always has a negative value. However, we assume that an eventual flow would be in the "z" direction. This avoids introducing vectors and allows us to only look at values.

$$\frac{dT}{dz} = \frac{-\alpha \cdot T \cdot g}{c_p} + \frac{(1-\alpha \cdot T) \cdot dp_{loss}}{\rho \cdot c_p} \tag{63}$$

Let's now consider the case where the fluid is incompressible ($\alpha = 0$) :

$$\frac{dT}{dz} = \frac{dp_{loss}}{\rho \cdot c_p} \tag{64}$$

In this case, the temperature can only increase (since $dp_{loss} < 0$) and depends only on the pressure loss. We clearly see here the irreversibility of the conversion of mechanical pressure energy into thermal energy.

The bias on the temperature gradient induced by the assumption of incompressibility is therefore of the order of $\frac{\alpha \cdot T \cdot g}{c_p}$.

Let's now consider the case where the pressure term is negligible in the enthalpy, i.e., $dH(T) = C_p \cdot dT$:

$$C_p \cdot dT + m \cdot g \cdot dz = 0 \tag{65}$$

$$\frac{dT}{dz} = \frac{-g}{c_p} \tag{66}$$

In this case, the temperature no longer depends on the pressure loss. It depends only on height.

The ongoing comparison of the approaches with OpenModelica is using a "DynamicPipe" component from the Modelica Standard library (MSL) coupled with a "pressure" sink at the pipe outlet (top part of the vertical pipe). The inlet conditions studied are of kind source of mass (and the necessary potential variables) flow and source of pressure (and the necessary potential variables).

5 Conclusion

This paper has addressed two key challenges in thermal-hydraulic system modeling: (1) the creation of a generic non-miscible liquid-gas medium that integrates with standard Modelica component libraries, and (2) the investigation of different approaches to model liquid incompressibility through detailed mathematical analysis.

The developed `BisubLiqGas` medium effectively represents systems that transition between fully liquid, fully gaseous, or mixed states, maintaining compatibility with standard components. This allows simulation of important scenarios like draining or leak management in systems such as Molten Salt Reactors. The model's generic structure enables adaptation to various liquid-gas pairs beyond the initial molten salt/helium application.

Our detailed mathematical analysis of different incompressibility approaches revealed significant implications for equation structure and numerical performance:

- The pure incompressible approach, while offering the simplest equation structure (algebraic pressure resolution), cannot model natural convection effects due to its constant density assumption.
- The semi-incompressible approach enables temperature-dependent density variations essential for buoyancy-driven flows, converting mass conservation into an explicit differential equation for temperature.
- The zero compressibility approach provides greater thermodynamic rigor but transform pressure resolution from algebraic to differential equations, increasing system complexity.
- The neglected pressure work variant offers numerical simplification but introduces thermodynamic inconsistencies that may affect accuracy in systems with significant pressure variations.

The theoretical analysis of vertical pipe flow demonstrated quantifiable differences between approaches. For instance, the temperature gradient bias induced by incompressibility assumptions is of the order $\frac{\alpha \cdot T \cdot g}{c_p}$, while neglecting pressure work in enthalpy leads to temperature gradients that depend solely on elevation rather than pressure losses.

This analysis revealed fundamental limitations of existing MSL `TableBased` media for implementing these approaches, particularly the counterintuitive behavior of the `singleState` parameter and the inability to represent zero compressibility formulations correctly. This justifies the development of specialized media rather than relying on generic table-based implementations.

These findings highlight the inherent trade-offs between physical accuracy and numerical efficiency in fluid modeling. The choice of incompressibility approach should be guided by the specific requirements of the application: natural convection modeling necessitates at least the semi-incompressible approach, while systems without significant buoyancy effects may benefit from the numerical advantages of the simpler incompressible model.

Future work will focus on implementing and validating these theoretical approaches in practical Modelica simulations, quantifying their performance differences in large-scale system models, and extending the analysis to more

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complex flow configurations. Additionally, exploring more sophisticated mixing rules for transport properties in the non-miscible medium would enhance the model's accuracy for specialized applications.

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