TAeZoSysPro: A Modelica Library for Thermal Aeraulic and Buildings Thermodynamics Calculations

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Abstract

TAeZoSysPro is a Modelica library developed for thermal and fluid dynamics simulations in industrial applications. The library provides components and models for heat transfer, fluid flow, and mass-energy release calculations. It includes modules for heat transfer modeling, fluid dynamics phenomena, specialized media, and partial differential equations. This paper presents the motivations behind developing this specific library and demonstrates its capabilities through industrial use cases, particularly for applications involving ventilation systems, equipment thermal behavior, and accident scenarios.
Keywords: fluid dynamics, heat transfer, Modelica, simulation, buildings thermodynamics

1 Introduction

The development of industrial systems relies increasingly on automated electrical equipment. In modern facility design, particular attention is paid to installation constraints, which has led to a higher concentration of thermal dissipation. This has highlighted new challenges related to thermal transients, especially in the event of ventilation loss.

Beyond these concerns, the TAeZoSysPro MODELICA library addresses another critical aspect: the impact of transients such as water/steam circuit breaches and boiling transients. These phenomena require detailed evaporation-condensation calculations and flexible modeling tools to effectively simulate installations, analyze transient behaviors, and perform sensitivity studies. For instance, (R. Moulouel et al. 2023) performed a sensitivity analysis on a nodal model to better understand how certain parameters influence the air temperature in an electrical room.

In the field of thermal modeling of buildings and industrial facilities, several Modelica libraries already exist, notably Buildings (Lawrence Berkeley National Laboratory 2025) and BuildSysPro (EDF R&D 2022). These libraries are primarily primarily designed for commercial building thermal systems. TAeZoSysPro positions itself as complementary by focusing on industrial thermal aspects and fine modeling of fluid dynamics phenomena. The library is compatible with the MODELICA Standard Library (Modelica Association 2021) interfaces and existing solutions while providing specific functionalities for industrial applications.

Recent studies (R. Moulouel et al. 2023) (Beiza et al. 2014) have emphasized the importance of accurately modeling thermal phenomena in industrial installations, particularly for predicting the behavior of temperature-sensitive equipment. However, existing libraries often lack specialized components that can address the complex thermal and fluid interactions typical of such environments.

The development of TAeZoSysPro was guided by several key requirements: accurate thermal modeling of industrial equipment such as electrical cabinets and transformers; implementation of the CARROLL method for improved separation of convective and radiative heat transfers; support for bi-species fluids, including handling of null species fractions and condensation phenomena; the capability to simulate transient thermal scenarios, such as ventilation loss; and full compatibility with existing Modelica libraries and the MODELICA Standard Library interfaces.

The present paper aims to provide a general overview of the TAeZoSyPro Modelica library which is available within the `OpenMODELICA` library manager or at https://gitlab.pam-retd.fr/TAeZoSysPro with detailed `html` description for each components. It first presents the theoretical foundations of the library, organized into two main subpackages: thermal heat transfer and fluid dynamics. For each subpackage, the main modeling assumptions are described and discussed in terms of their implications and limitations. Key components are illustrated to convey the overall modeling philosophy. Finally, typical application examples are presented, including comparisons with experimental results when available.

2 Library Overview

TAeZoSysPro is organized into four main modules as illustrated on Figure 1 and detailed further in the following subsections.

2.1 Heat Transfer

This module provides components for modeling heat transfer through conduction, convection, and radiation. It includes models for walls, equipment, and thermal exchanges with the environment. Built on a nodal approach, the module enables a detailed and flexible representation

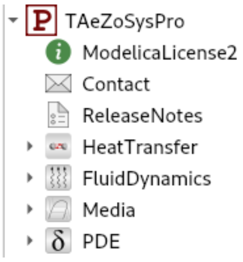

Figure 1. TAeZoSysPro library general architecture

of thermal phenomena.

2.2 Fluid Dynamics

This module handles air flows and mass-energy transfers, enabling the simulation of evaporation-condensation phenomena and multi-species flows. A key feature is the ability to model phase changes, which are essential for capturing a wide range of industrial thermal processes.

2.3 Media

The Media module defines the thermodynamic properties of fluids used in the library, with particular attention to bi-species mixtures and condensation phenomena. The module implements specialized materials whose properties vary with temperature, pressure, and composition. Unlike the standard Modelica Media library, TAeZoSysPro media can handle null species fractions, which is crucial for certain industrial scenarios such as pool boiling, where non-condensable species (e.g., air) are initially present and gradually replaced by steam during the boiling transient.

2.4 PDE

This module provides tools for solving partial differential equations (PDEs), enabling detailed modeling of physical phenomena. It supports spatial discretization schemes tailored to specific types of transport processes and is designed to be used as a subcomponent within more complex systems. The module includes a first-order upwind 1D spatial discretization scheme for purely advective transport, and a second-order centered 1D spatial discretization scheme for diffusive transport. Temporal discretization is handled directly by the Modelica solver used in the simulation environment. Temporal discretization scheme is directly handled by used Modelica solver. The module solves advection-dominated transport equations of the form:

$$\alpha \partial_t Y + \beta \partial_x Y = \dot{\omega} \tag{1}$$

Here, α and β are constants across the spatial domain, specified by the modeler. $\dot{\omega}$ is a source term that can vary from node to node, and Y represents the transported quantity (e.g., enthalpy). Typically, $\alpha = \rho$ and $\beta = \rho U_b$ for a dynamic pipe where U_b stands for the bulk velocity within the pipe. The module also supports diffusion-dominated transport described by:

$$\alpha \partial_t Y = \gamma \partial_{x^2} Y + \dot{\omega} \tag{2}$$

In this case, γ is the diffusion coefficient. The same conventions apply for α, $\dot{\omega}$, and Y as in the advection case.

3 General framework

All physics model embedded in the library are based on the three fundamentals balance equations of the Navier-Stokes equations which are conservation of mass, conservation of motion and conservation of energy. The first rely on mass conservation, the second is establish using the Newton second law while the latter is established with the first principle of thermodynamics:

$$\partial_t \rho + \underline{\nabla} \cdot (\rho \underline{u}) = 0 \tag{3}$$

$$\partial_t (\rho \underline{u}) + \underline{\nabla} \cdot (\rho \underline{u} \otimes \underline{u}) = -\underline{\nabla} p + \underline{\nabla} \cdot \underline{\underline{\tau}} + \rho \underline{g} \tag{4}$$

$$\partial_t (\rho e_t) + \underline{\nabla} \cdot (\rho \underline{u} e_t) = \underline{\nabla} \cdot \left(\underline{u} \cdot \underline{\underline{\sigma}} \right) + \rho \underline{u} \cdot \underline{g} - \underline{\nabla} \cdot \underline{q} + \dot{\omega} \tag{5}$$

where ρ is the density, $\underline{u}$ the velocity, μ the kinematic viscosity, p the pressure, $\underline{g}$ the gravity, $\underline{\underline{\sigma}}$ the stress tensor, e_t the total energy, q the heat flux, $\dot{\omega}$ the volumetric heat gain. The stress tensor can be decomposed as follow:

$$\underline{\underline{\sigma}} = \underline{\underline{\tau}} - p \underline{\underline{1}} \tag{6}$$

where $\underline{\underline{\tau}}$ is the viscous stress tensor. The total energy e_t can be decomposed as the sum of the internal energy and the kinetic energy.

$$e_t = e + \frac{1}{2} u^2 \tag{7}$$

In zonal approaches, local equations previously defined are generally integrated over a large volume of control defined by physical boundary such as a whole pipe, a room or a vessel. Effects of unresolved small scales needs then to be adequately accounted at the resolved scales level, usually relying on relevant correlations. The following subsection presents how local balances are integrated and solved within the TAeZoSysPro modelica library.

3.1 Heta transfer sub-package approach

Objective of this sub-package is to solve the energy equation 5 integrated over the whole volume of components used to model the studied system. A balance of kinetic energy is performed by multiplying Equation 4 on both side by $\underline{u}$ and substitute to Equation 5 leading to:

$$\partial_t (\rho e) + \underline{\nabla} \cdot (\rho \underline{u} e) = -\underline{\nabla} \cdot \underline{q} + \dot{\omega} + \mu S^2 - p \underline{\nabla} \cdot \underline{u} \tag{8}$$

where $S^2 = \underline{\underline{\tau}} : \underline{\underline{\tau}}$ is dissipated kinetic energy power due to fluid viscosity which is generally neglected. The enthalpy $h = e + p/\rho$ is introduced in Equation 8. Assuming constant pressure transformation, incompressible flows and constant specific heat c_p, enthalpy can be expressed as $h = c_p T$ and Equation 8 reads:

$$c_p \partial_t \rho T + c_p \underline{\nabla} (\rho \underline{u} T) = -\underline{\nabla} \cdot q + \dot{\omega} \tag{9}$$

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Integration of this latter equation over a volume of control, denoted c, whose mean temperature is defined as:

$$T_c = \frac{1}{m_c} \iiint_V \rho T dV \tag{10}$$

leads to:

$$V_c \rho_c \partial_t T_c - \dot{W} = \sum_i \dot{m}_i c_p (T_i - T_c) + \sum_j \Phi_j \tag{11}$$

where Φ_j is the thermal flux at the boundary j of the control volume, $\dot{m}_i$ the mass flux at the boudary i and $\dot{W}$ the total heat gain at the component level volume which can eventually account for thermal radiant transfers absorption. For each boundary with inlet mass flux, flow being assumed incompressible, a boundary with exactly the mass flux exists assuming leaving temperature is the mean component temperature. Within the thermal sub-package, mass fluxes are considered as model parameters that needs to be provided by the modeler, the only state variable of models only constructed with this sub-package is thus the temperature T.

Elementary components assembly rely on a staggered scheme, as illustrated on Figure 2, where state variables are computed within capicity components, the nodes, with time derivative ∂_t and fluxes between inertial components are computed within fluxes components based on connected state variables values. Typically, left hand side of Equation 11 is handled in capacity components while right hand side is handled within flux components.

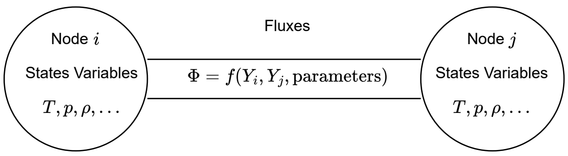

Figure 2. Staggered scheme between nodes

Thermal fluxes at component boundaries can involve radiant, convective, or conductive transfers. Convective heat transfers at a solid-fluid boundary refer to the conductive heat fluxes at the wall, which are then carried away by the fluid motion within the boundary layer. Conductive heat fluxes are accounted using Fourrier's law:

$$\phi_{cond} = -\lambda \underline{\nabla} T \tag{12}$$

where λ is the thermal conductivity. Convective fluxes are estimated using Newton's cooling law:

$$\phi_{cv} = h_{cv}(T_w - T_c) \tag{13}$$

where T_w is the wall surface temperature and h_{cv} is the heat transfer coefficient which have to either provided by the modeler or estimated using correlation in the typical form $Nu = f(Ra, Pr)$ with Nu being the Nusselt number, Ra the Rayleigh number and Pr the Prandtl number.

Radiant heat fluxes between surfaces can be either modeled with radiant heat exchange coefficient h_r to be added to h_{cv} or with a fictive mean radiant node, denoted the Carroll node, as exposed by (Carroll 1980). In this context, the radiosity of the Carroll node is:

$$J_{MRT} = \frac{\sum_k F_k J_k S_k}{\sum_k F_k S_k} \tag{14}$$

where k relates to the k^{th} opaque surface involved with S_k surface, J is the radiosity and F_k is the Carroll surface viewing factor. This latter factor is computed using the following heuristic equation:

$$F_i = \frac{1}{1 - \frac{S_i F_i}{\sum_k F_k S_k}} \tag{15}$$

The net radiant fluxes for each involved opaque surface is then estimated as follow:

$$\phi_{rad} = F_i' \left(J_{MRT} - \sigma T_i^4 \right) \tag{16}$$

where σ is the Stefan-Boltzmann constant and F' the viewing factor modified to account emissivity of surface.

$$\frac{1}{F_i'} = \left(\frac{1 - \varepsilon_i}{\varepsilon_i} + \frac{1}{F_i} \right) \tag{17}$$

This approach is applied to each components, such air volume control, slice of walls or isothermal mass, for each them boundary fluxes needs to be modeled with relevant approaches to account thermal conductive fluxes within the unresolved boundary layer.

3.2 Fluid dynamics sub-package approach

Fluid dynamics aims to solve the three fundamental balance equations—mass conservation (3), momentum conservation (4), and energy conservation (5)—at an integral scale level by integrating them at the level of macroscopic components with physical boundaries.

A staggered approach, depicted in Figure 2, is also applied within this module. The node modeled within this package can handle mixtures of species, including possible condensation.

Mass conservation is solved for each species, while global equations for the conservation of momentum and energy are solved. Equations of state for each species enable the system to be closed. In defining the number of equations solved, the equations of state are usually not counted. Therefore, the Fluid Dynamics Package is commonly referred to as a model with four equations in the case of humid air, which is the primary focus of this module.

Integration of mass conservation for each species leads to:

$$\partial_t m_i = \sum_j \dot{m}_i + \Gamma_i \tag{18}$$

where $\dot{m}_i$ are the mass fluxes for the species $_i$, Γ_i is the mass generation (can be negative) of a given species which can be due to phase change leading to drain vapor from humid air because of condensation for instance. Within each node, mean temperature T_c is assumed to be the same for each species while pressure and density is computed as follow:

$$p = \sum_i p_i \quad \rho = \sum_i \rho_i \quad e = \sum_i X_i e_i \quad X_i = \rho_i / \sum_i \rho_i \tag{19}$$

where X_i is the mass fraction of species i.

Mass fluxes at fluid interfaces are estimated by assuming a ratio between the Nusselt number and the Sherwood number close to one ($Nu/Sh \approx 1$). Additionally, the Lewis number ($Le = \alpha/D$), where α is the thermal diffusivity and D is the mass diffusivity, is also assumed to be close to one. This allows for the definition of the mass transfer coefficient and the associated mass flux as follows:

$$h_m = \frac{h_{cv}}{c_p} \tag{20}$$

$$\phi_m = h_m (X_w - X_c) \tag{21}$$

where X_w is the mass fraction of the species at the wall, which is assumed to be equal to the saturated mass fraction as a maximum.

Conservation of momentum energy is integrated between node, within equivalent pipes or duct of section S using Bernouilli's theorem which can be derived from Equation 4 for incompressible and irrotational flow. The fluid head is then defined as:

$$H = p + \frac{1}{2}\rho u^2 + \rho g \tag{22}$$

Within an equivalent pipe the integral solve equation is:

$$\underbrace{S_p L_p \rho_m \partial_t u_b}_{\text{unsteady term}} + \underbrace{S_p \left[(p_o + \rho_m g z_o) - (p_i + \rho_m g z_i)\right]}_{\text{head flux integral balance}} = \underbrace{S_p \Delta H}_{\text{singular and regular head losses}} \tag{23}$$

where u_b is the bulk velocity, ρ_m is the mean fluid density within pipe, z the altimetry, L_p its length and S_p its cross section surface. $_i$ stands for pipe inlet and $_o$ for pipe outlet. S_p is assumed to be the same at pipe inlet and outlet, implying and equal dynamic pressure at the inlet and the oulet, however singular head losses due to singularities such as pipe diameter change can be accounted in the singular head losses term. The flow within pipes is assumed to be quasi static regarding mass balance equation, the mass flux within pipe is thus:

$$\dot{m}_p = u_b \rho_m S_p \tag{24}$$

Within each node, only the total pressure defined as $p_t = p + 1/2\rho u^2$ and the total energy are used within balance equation.

The energy conservation equation 5 is integrated at the node level neglecting the work of the viscous forces at the boundaries $\underline{\nabla} \cdot \underline{\underline{\tau}}$ and the work of the volumes forces $\rho \underline{u} \cdot \underline{g}$. One can notice that work of the pressure force can be combined with the advection of internal energy:

$$\underline{\nabla} \cdot (\rho \underline{u} e) + \underline{\nabla} \cdot \left(\underline{u} \cdot p \underline{\underline{1}}\right) = \underline{\nabla} \cdot (\rho \underline{u} h) \tag{25}$$

where $h = e + p/\rho$ is the enthalpy. At the node level, the resulting balance is:

$$V_c \partial \left(\rho_c e_{c,t}\right) - \dot{W} = \underbrace{\sum_i \dot{m}_i h_i}_{\text{enthalpy fluxes}} + \underbrace{\sum_j \Phi_j}_{\text{heat fluxes}} \tag{26}$$

3.3 Moist air media

Theory presented in §3.1 and §3.2 is valid for any media within the volume control. Thermodynamics properties are computed separately within the TAeZoSysPro library to enable the use of the `Media` packages of the `Modelica Standard Library` if needed. The library has a specific media dedicated to moist air, with a formulation based on temperature and density (ρ, T) as explicit variables to handles potential total disappearance of one species while still being numerically stable. The enthalpy of the fluid is estimated as the ratio of the different mass fraction X:

$$\begin{aligned} h = {} & X_a \underbrace{c_{p,a}(T - T_{ref})}_{\text{dry air enthalpy}} \\ & + X_v \underbrace{\left[c_{p,wv}(T - T_{ref}) + h_{vl}(T_{ref})\right]}_{\text{vapour enthalpy}} \\ & + X_l \underbrace{c_{p,wl}(T - T_{ref})}_{\text{liquid water enthalpy}} \end{aligned} \tag{27}$$

where $h_{vl}(T_{ref})$ is the latent heat of water at the reference temperature. The mass fraction of liquid water within a node is computed as a function of the saturation density $\rho_{sat} = f(T)$ ensuring ρ_{wv} is below the saturation density. The fraction of liquid water within a gas node is expected to be small but possible, for instance, in the case of fog. Specific nodes for this medium are available in the library to manage the drainage of liquid from the node. This is based on the fall speed of water droplets and the a priori number of droplets per unit of volume.

4 Heat Transfer Details

4.1 Bases classes subpackage

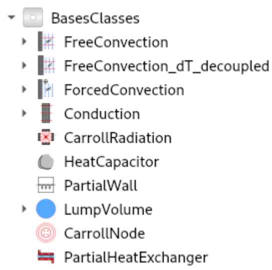

Figure 3. BasesClasses TAeZoSysPro subpackage overview

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The `BasesClasses`, illustrated in Figure 3, subpackage includes elementary functions that can be used directly within a model or serve as building blocks for more complex macro components.

Ports used by components within this package involve only on one state variable declared as follow:

Listing 1. Thermal port for heat transfer appoach

```
within TAeZoSysPro.HeatTransfer.Interfaces;

partial connector HeatPort "Thermal port
    for 1-dim. heat transfer"
  Modelica.SIunits.Temperature T "Port
      temperature";
  flow Modelica.SIunits.HeatFlowRate Q_flow
```

These ports are fully compatible with the thermal port defined in the Modelica Standard Library as well as in BuildSysPro (EDF R&D 2022)

4.1.1 Convection

Several correlations are available to handle various free and forced convection scenarios encountered in industrial installations, including vertical walls, ceilings, ground surfaces, and cylinders. These correlations are used to compute the Nusselt number (Nu), from which the convection coefficient is determined using the relation $h_{cv} = Nu\lambda/L_c$. Alternatively, this coefficient can also be directly specified by the user. The heat convection flux is then computed using Equation 13.

4.1.2 Conduction

For conduction through a homogeneous material, the heat conduction flux modeled using Fourier's law (Equation 12). In practice, the PDE module is typically used to solve the heat equation for a wall with a given thermal conductivity by discretizing the wall into multiple layers or nodes.

4.1.3 Carroll Radiation

This component implements the Carroll radiation method, as detailed in subsection 3.1. It is associated with each radiative surface, for which the area and emissivity are specified, and is connected to the `CarrollNode`. Additionally, it interfaces with the `FviewCalculator`, which computes and supplies the Carroll view factor, accounting for the configuration of all radiative surfaces.

4.1.4 Elementary components

In addition to the previously introduced functions for handling various modes of heat transfer, the `BasesClasses` subpackage includes elementary components such as the `HeatCapacitor`, which is characterized by a given mass and thermal capacitance and allows for the supply of a heat flux. The `LumpVolume` component models the thermal inertia of an open lumped volume by linking variations in potential enthalpy (or temperature for an ideal gas) to the heat flow balance. It operates under the assumption of constant pressure and accounts for isobaric expansion, as the volume boundaries are not sealed.

4.2 Main Components

The library provides several basic components for thermal and basic HVAC modeling:

- `Wall`: models walls with consideration of thermal inertia and homogeneous material (an special multilayer wall model is also available). The wall model solves the heat equation with appropriate boundary conditions using the PDE module assuming 1-D thermal conduction:
- `InertMass`: represents equipment thermal masses with a lumped thermal capacity:

$$C \cdot \frac{dT}{dt} = \sum \dot{Q}_{in} - \sum \dot{Q}_{out} \quad (28)$$

  where C is the thermal capacity, T is the temperature, and $\dot{Q}_{in}$ and $\dot{Q}_{out}$ are the incoming and outgoing heat flows.
- `HeatExchanger`: models heat exchangers using an effectiveness approach:

$$\dot{Q} = \varepsilon \cdot C_{min} \cdot (T_{h,in} - T_{c,in}) \quad (29)$$

  where ε is the effectiveness, C_{min} is the minimum heat capacity rate, and $T_{h,in}$ and $T_{c,in}$ are the inlet temperatures of the hot and cold fluids.
- `Ventilation` and `FanVentilation`: simulate ventilation systems with variable flow rates and temperature influences.
- `FviewCalculator`: implements the CARROLL method to calculate radiative temperatures and view factors for radiative exchanges. This component is a key element in the library's approach to radiation modeling. It computes view factors between surfaces without requiring detailed geometric information, using only the surface areas as inputs.
  The CARROLL method creates a virtual node (represented by the `CarrollNode` component) that acts as a fictitious blackbody enclosure exchanging radiation with all surfaces. This node's temperature corresponds to the Mean Radiant Temperature (MRT).
- `CabinetPower`: a significant example of a macro component is the model, which represents an electrical cabinet with its thermal dissipations. Having a RealInput port connection for the heat power allows for a fine control of the thermal power dissipated by the cabinet, including transient behaviors.
  The model solves a system of equations for each thermal node representing the emitter inside the cabinet and the casing of the cabinet. The heatload are dissipated within the emitter. The emitter exchanges by convection with the fluid between the emitter and the casing. Regarding the convection, the emitter is supposed flat and horizontal or vertical depending on the value of `correlation_internal`. The convective surface of the emitter (*A_conv_emitter*) has thus

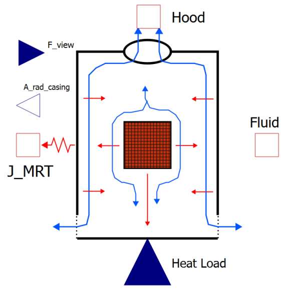

Figure 4. Icon view of the CabinetPower model

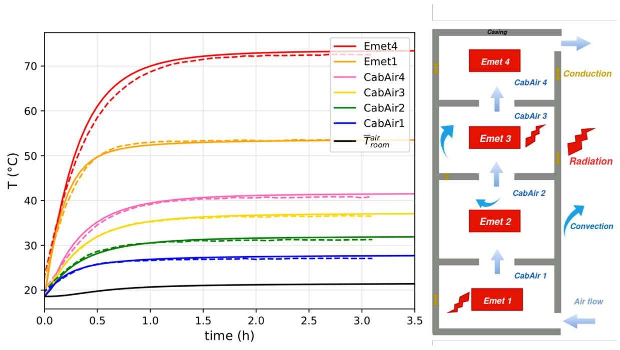

Figure 5. Comparison of the Zephyr electrical cabinet model with experimental data

to be an equivalent surface is both vertical and horizontal surfaces are present. For the casing for the inner and outer convection, the correlation is always a correlation for a vertical plate.

Based on the `CabinetPower` model, a more detailed representation can be developed to investigate various physical phenomena. For instance, the model of the electrical cabinet room (cf. Figure 6) reproduces the actual experimental setup: a simple parallelepiped cabinet with four vertically stacked drawers. Each drawer is represented as an enclosing structure containing a mass-based heat emitter. These emitters exchange heat via radiation with the cabinet's enclosure and through natural convection with the air inside the drawers. The enclosure, in turn, exchanges heat by convection with the ambient room air and by radiation with Carroll's radiosity node (MRT). Additionally, the cabinet features openings that enable air circulation between the drawers and with the room's aeraulic node. This detailed electrical cabinet model was calibrated and validated using experimental data shown in Figure 5.

4.3 Application Example: Room with Electrical Cabinet

In order to study thermo-aeraulic phenomena in industrial spaces containing thermosensitive electrical equipment, EDF-R&D has developed a dedicated experimental facility within the ZEPHYR laboratory (Rafik Mouloue1 et al. 2024). This full-scale, instrumented facility, shown in Figure 6 is representative of the electrical or control-command rooms found in nuclear power plants. It allows detailed temperature fields measurements to be taken in the air and in the surrounding walls under controlled and repeatable conditions, making it suitable for validating numerical simulation models.

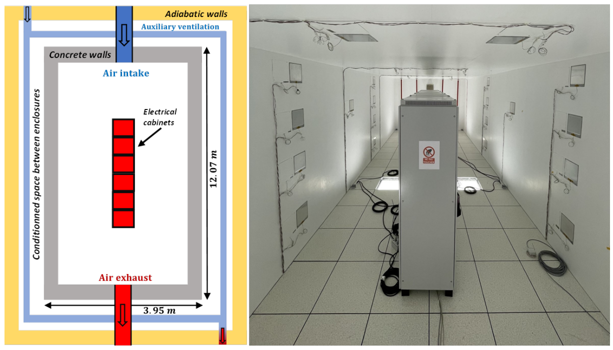

Figure 6. Picture of the electrical cabinets room facility

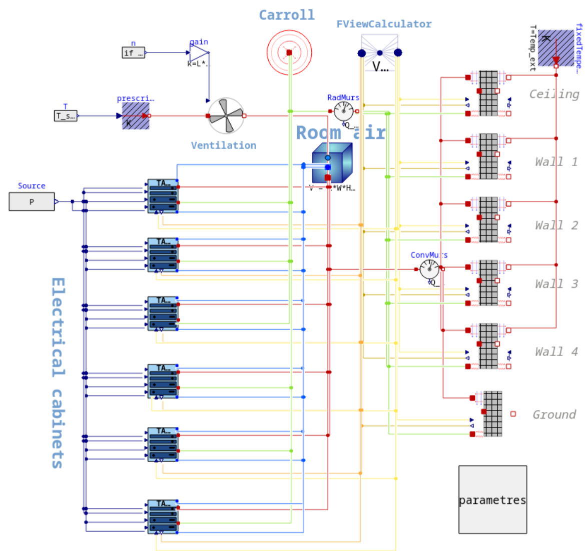

Figure 7. TAeZoSysPro model of the Zephyr electrical room cabinet facility

This experimental cell was modeled using the TAeZoSysPro library, as illustrated in Figure 7, to investigate its behavior and perform sensitivity analysis (R. Mouloue1 et al. 2023). The thermal interactions between the cabinets and their surrounding environment were simulated, along with the air circulation within the various compartments of the cabinets. The influence of the ventilation and the external conditions were studied. Multiple experiments, varying several thermo-aeraulic parameters, were conducted. The results were then compared to both a CFD model and the TAeZoSysPro model, as shown in Figure 8. The 3-D modeling is implemented using the OpenSource CFD solver Code Saturne((Archambeau, Méchitoua, and Sakiz 2004), (EDF 2021)). This comparison demonstrates the TAeZoSysPro library's capability to predict air temperature, although it tends to overestimate it due to its assumption of a homogeneous temperature across the entire room volume, which does not account for thermal strati-

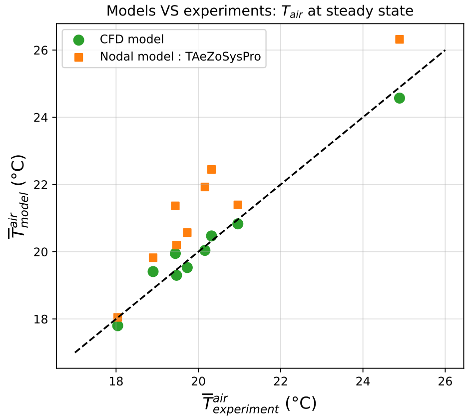

Figure 8. Comparison of TAeZoSysPro thermo-aeraulic model prediction to experimental data

fication. In contrast, the CFD model provides a more accurate prediction of the average air temperature at steady state. These findings will be discussed in further publications.

4.4 Current Limitations

The current approach of separating radiative exchanges presents certain limitations, particularly in the absence of thermal stratification modeling. While the CARROLL method provides advantages for detailed analysis of radiative phenomena, the lack of a stratification model can lead to less accurate results in some scenarios. Developments are ongoing to improve the modeling of these phenomena.

5 Fluid Dynamics Details

The fluid dynamics package is organized in a similar way as the heat transfer package described in §4 and illustrated on Figure 9. Each node is provided

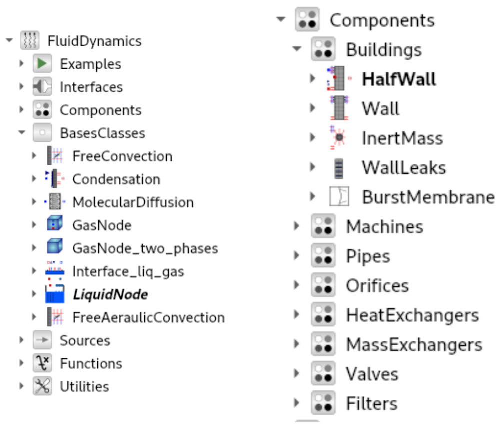

Figure 9. Overview of the fluid dynamics module

with three `Modelica` ports. One Thermal port presented on Listing 1 to handle heat fluxes, a `flowPort` dedicated to moist air media presented in §3.3 and a `Modelica.Fluid.Interfaces.FluidPort` to ensure compatility with the Modelica Standard Library.

Listing 2. FlowPort port for Fluid Dynamics module

```
within TAeZoSysPro.FluidDynamics.Interfaces
    ;
connector FlowPort "Connector flow port"
  replaceable package Medium = Modelica.
      Media.Interfaces.PartialMedium "
      Medium model" annotation(
    choicesAllMatching = true);
  Medium.Temperature T;
  Medium.Density[Medium.nX] d;
  flow Medium.MassFlowRate[Medium.nX]
      m_flow;
  flow Modelica.SIunits.EnthalpyFlowRate
      H_flow;
```

5.1 Specialized Media

The library implements two specific media models.

- **Moist Air Media** - For mass-energy release calculations ;
- **Air H2 Media** - As an example media to track a specific species.

The moist `MoistAir` is a specialized model using density and temperature as explicit state variables, which handles the phase transition between vapor and liquid water with superior numerical stability. A Generic bi-species mixtures, providing a framework for modeling various fluid combinations is also proposed.

The `MoistAir` model in TAeZoSysPro is formulated with density and temperature (ρ, T) as primary state variables, unlike other implementations that use pressure and temperature or enthalpy and pressure. This explicit formulation offers several significant advantages:

- **Enhanced numerical stability** - Particularly important during phase transitions where pressure may experience discontinuities, while density varies more continuously
- **Better handling of near-saturation states** - The (ρ, T) formulation facilitates calculations in regions near saturation, where property derivatives with respect to pressure can become very large
- **Direct mass conservation calculations** - Mass conservation equations are directly expressed in terms of density, simplifying the differential equations to be solved
- **Smoother phase transitions** - Special numerical treatments manage state transitions without the discontinuities that can lead to simulation failures

A key difference between TAeZoSysPro media and the standard `Modelica.Media.Air.MoistAir` is the ability to handle null species fractions. In the standard MSL implementation, having zero mass fraction of a species can lead to numerical issues in certain calculations. TAeZoSysPro implements robust handling of these edge cases, ensuring continuous simulation even when a species disappears completely due to phase change which can be typically the case in industrial buildings thermodynamics studies.

Additionally, the condensation model in TAeZoSysPro includes special numerical treatments to handle the transition between states smoothly, avoiding the discontinuities that can cause simulation failures in complex systems.

5.2 Main Components

An overview of some of the main components is presented below, though it is not exhaustive. The required media are declared as `Replaceable Package` within each component and subcomponent to allow the modeller to use any medium compatible with the proposed structure of the Modelica Standard Library.

The component `gas_node_two_phases` implements mass and energy conservation equations while allowing for phase changes of condensable species and drain of condensate based on fall velocity of liquid droplets. This component is specific to the TAeZoSysPro MoistAir Media.

The `condensation` elementary component model the mass flow rate and energy transfer induced by the condensation of a condensable species over a colder surface. The component is used on macro components such as wall dedicated to studies with potential condensation. In case of surface temperature below dew point, it is assumed that water vapour density within the boundary layer is equal to the saturation density estimated with the wall temperature. Mass transfer flowrate is computed using mass coefficient defined in §3.2.

`Interface_liq_gas`: This component models a flat interface between liquid and surrounding gas where evaporation-condensation, boiling, radiation, and convection occur. It is designed to work with the TAeZoSysPro moist air media for the gas media and Standard Water of the `MSL` for the liquid media. *Evaporation-condensation* is modelled with a similar approach than condensation on surface. Evaporation occurs is liquid surface saturation density is higher than water vapor density in the connected gas node. *Convection* and *Radiation* are modelled with the approach presented in §3.1 *Boiling* is modelled as homogeneous formation of equal-diameter bubbles that form in the liquid node and escape through the interface The boiling process is modeled thanks to the estimation of the gas fraction within liquid node from the dew and buble enthalpy when the fluid enthalpy is higher than bubble enthalpy but lower than dew point enthalpy:

$$h = (1 - X_g)h_{bubble} + X_g h_{dew} \tag{30}$$

where X_g is the gas mass fraction within the connected liquid node.

The library propose also flow junctions and separations, allowing for complex network modeling. A set of heat exchangers with phase change, which handle energy transfer between fluids while accounting for condensation or evaporation is available, which is particularly valuable for building thermodynamics or cooling coils studies.

A subpackage containing walls and building orifices is dedicated to components needed for building thermodynamics studies, typically involving vapor breaches.

These components are interconnected to model complex fluid systems with multi-species flows and phase changes. The module implements a connector-based approach, where connectors carry information about pressure, mass flow rate, enthalpy, and species composition.

5.3 Applications

Two application cases illustrate the library's capabilities:

5.3.1 Pressure Cooker Model

This example case validates the modeling of evaporation phenomena under pressure:

- Pressure rise through evaporation, following the relationship between temperature and saturation pressure
- Liquid-vapor thermodynamic equilibrium, ensuring consistency between phases
- Pressure regulation through relief valve, modeling the mechanical behavior of the system

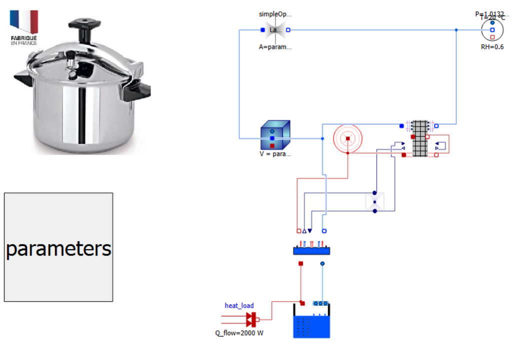

Figure 10. Model of a pressure cooker

The Modelica implementation of this model integrates the following key components:

- A two-phase gas node (`gasNode_two_phases`) representing the steam phase above the liquid
- A liquid node (`liquidNode`) modeling the water volume with thermal inertia
- A liquid-gas interface (`interface_liq_gas`) that handles mass and heat transfer between phases
- A vessel wall (`wall`) with thermal inertia and heat transfer capabilities
- A simple opening component (`simpleOpeningComp`) acting as a pressure relief valve
- A heat source (`heat_load`) providing 2000 W of thermal power to the system
- A Carroll node (`carrollNode`) implementing the CARROLL method for radiative heat transfer calculations

The model uses the `MoistAir` medium from TAeZoSysPro's Media library, which handles the water-vapor mixture with phase change capabilities. Key parameters include the total volume (`V_tot`), gas phase volume

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(V_gas), wall surface area (S), interface area (A), and thermal properties such as emissivity (eps).

This model demonstrates the library's ability to handle phase changes and pressure dynamics in a closed system. The resulting pressure and temperature curves match experimental data, confirming the accuracy of the phase change calculations.

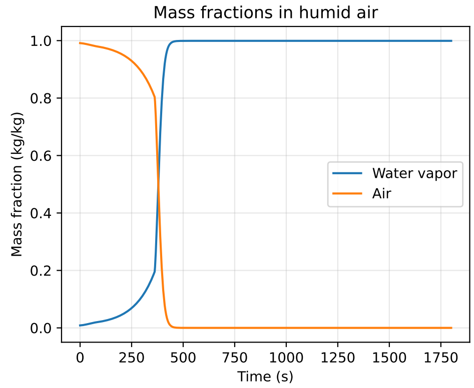

Figure 11. Evolution of mass fractions in the pressure cooker model.

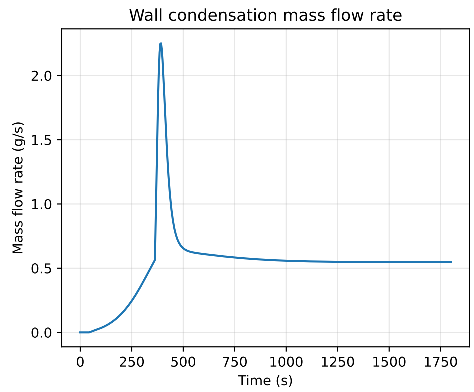

Figure 12. Condensation mass flow rate on the inner wall of the pressure cooker.

The simulation results illustrated in Figures 11 and 12 highlight several key phenomena that occur during the pressure cooker heating process:

- **Phase transition dynamics**: As shown in Figure 11, we observe the gradual evolution of species composition in the gas phase, with a continuous decrease in air mass fraction counterbalanced by an increase in water vapor fraction. This transition demonstrates how the model captures the progressive replacement of incondensable air by water vapor during heating.
- **Condensation phenomena**: Figure 12 illustrates the mass flow rate of condensation occurring at the inner wall of the pressure cooker. The initial peak corresponds to the early heating phase when temperature differences between the vapor and the cooler wall are significant, followed by variations that reflect the complex thermal equilibrium establishment.
- **Multi-phase interactions**: The combined analysis of both figures reveals the interplay between evaporation at the liquid-gas interface and condensation at the cooler walls, showing how the model accurately represents the complete cycle of water phase changes in a confined environment.

These results validate the library's capability to simulate the complex thermodynamic behavior of multi-species fluids undergoing phase changes, a critical feature for industrial applications involving pressurized systems and heat transfer.

5.3.2 Boiling and Steam Line Breaches Transients

A second application case concerns the simulation of transients in nuclear power plant scenarios, including high energy breaks (water/steam line breaches) and pool boiling phenomena (such as in spent fuel pools). These simulations allow for the observation of impacts on pressure and temperature in containment rooms, taking into account various physical phenomena:

- Progressive liquid evaporation and condensation processes, with bidirectional mass transfer between phases
- Thermodynamically-driven phase changes, calculated based on local conditions and interface properties
- Heat transfer through multiple mechanisms (conduction, convection, radiation) affecting phase transition rates and wall temperature
- Pressure increase dynamics resulting from vapor generation and gas compressibility effects
- Spatial distribution of thermal effects and resulting flow patterns

The model Figure 13 captures the complex coupled behavior between thermal, fluid dynamic, and phase change phenomena, providing detailed insights into the evolution of temperature, pressure, humidity, and phase composition during accident scenarios. This capability is particularly valuable for safety analyses where accurate prediction of containment conditions is essential.

This model demonstrates the library's ability to handle phase changes and pressure dynamics in a closed system. The resulting pressure Figure 14 and temperature curves match experimental data, confirming the accuracy of the phase change calculations. Results have been compared against experimental data including the Carolinas-Virginia Tube Reactor (CVTR) containment response tests (Schmitt, Bingham, and Norberg 1970), which provided valuable benchmark data for evaluating steam condensation models under conditions representative of containment structures in nuclear power plants. The initial comparisons are encouraging and show a reasonable level of agreement and a behaviour representative of the experimental data. Some discrepancies are observed in the pressure curve, which is likely due to the complex geometry of the CVTR containment structure and the associated modeling bias.

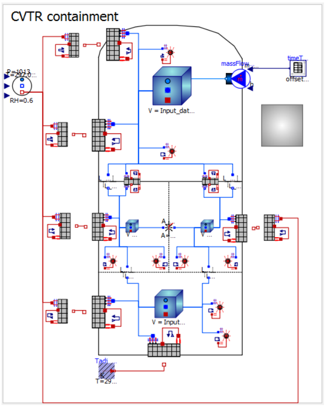

Figure 13. TAeZoSysPro model of the CVTR containment structure.

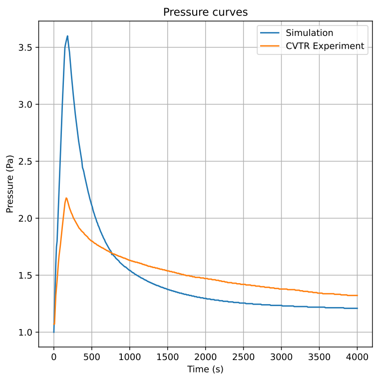

Figure 14. Comparison of pressure evolution between TAeZoSysPro simulation and CVTR experimental data.

6 Conclusion and Perspectives

The TAeZoSysPro library provides an innovative solution for modeling thermal and aeraulic phenomena in industrial installations including buildings thermodynamics. Its strengths include:

- Fine modeling of heat transfers with the CARROLL method and convective heat transfer correlations allowing separating convective and radiative phenomena
- Building Thermodynamics calculations using advanced management of bi-species media with robust handling of null species fractions and condensation
- Experimentally validated components
- Modular architecture, standard interfaces facilitating extensions and coupling with other libraries

Future developments will focus on:

- Improvement of thermal stratification models
- Extension of validation cases
- Qualification of the library according to industrial standards
- Implementation of automatic non-regression tests and MODELICA validation tests allowing the qualification files to be up to date with the latest version of the library
- Extension of multi-scale modeling capabilities

Finally, the modular design of TAeZoSysPro makes it particularly suitable for coupling with uncertainty propagation tools like OpenTURNS (OpenTURNS Team 2023), enhancing its utility for industrial applications where understanding parametric sensitivities is crucial.

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