Integral Analysis for Thermo-Fluid Applications with Modelica

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Abstract

Integral analysis is a common technique used in the solution of many thermo-fluid problems. While previous applications of integral analysis techniques focused on the solution of boundary layer problems, the techniques are applicable to a wider range of analyses. This paper describes a formulation in Modelica for integral analyses in thermo-fluid applications. Following a brief overview of integral analysis, a sample Modelica implementation is discussed along with numerical simulations that illustrate the model usage in thermo-fluid applications. Additional applications and usage scenarios of the integral analysis formulation are briefly discussed.

Keywords: integral analysis; thermal; fluid

1 Introduction

Heat transfer and fluid flow phenomena are governed by partial differential equations (PDEs) for conservation of mass, momentum, and energy. There are no general, closed-form solutions for these coupled, nonlinear PDEs. While analytic solutions are available for a small class of problems with special boundary conditions, more general analyses with PDEs require numerical approaches, such as discretization and differencing, to resolve the spatial and temporal dynamics.

In contrast to the PDE approach, lumped parameter modeling is formulated by conservation of spatially-integrated quantities. Thus, the temporal dynamics in the relevant conservation equations are retained resulting in ordinary differential equations (ODEs) for the conservation laws of a lumped control volume. It is still possible to obtain spatial dynamics with lumped parameter models by explicitly introducing networks of control volumes. Lumped parameter models typically are relatively easy to formulate, computationally-efficient, and can use standard ODE numerical solvers for simulation. The Modelica `Thermal` library [1] is a lumped parameter formulation for heat transfer, and Modelica has been used extensively in thermo-fluid applications (*c.f.* [2]-[5]).

In applications where spatial resolution is important, a hybrid modeling approach that combines aspects of the PDE and lumped parameter formulations may be appropriate. Integral analysis is one such technique that has been used to solve a variety of thermal and fluid problems [6]. The integral analysis technique was first proposed by von Karman [7] and Polhausen [8] for boundary layer solutions and is sometimes referred to as the Von Karman-Polhausen method. This method has been used extensively for boundary layer problems [9] and provides reasonably accurate results when compared with the exact solutions of the governing PDEs with considerably less computational expense and complexity. Integral analysis typically involves the following steps:

- Casting the governing PDEs in integrated form
- Choosing representative spatial profiles with unknown coefficients for the appropriate variables (usually temperature and velocity in thermo-fluid problems)
- Solving for the coefficients as a function of the relevant boundary conditions

This technique can be used for both transient and steady state problems and provides the benefits of a lumped parameter formulation with some additional information regarding spatial distribution without resorting to the solution of PDEs.

This paper describes the implementation of an integral analysis formulation for thermo-fluid applications in Modelica. To illustrate the steps for deriving an integral analysis formulation, sample formulations for various geometries are shown along with example problems illustrating the approach in numerical simulations for simple thermal and thermo-fluid problems with conduction and convection heat transfer. More advanced applications of the resulting models for combined heat and mass transfer simulations are illustrated via a model of heat exchanger fouling.

2 Integral Analysis Formulation

This section outlines an integral analysis formulation for thermal problems. It should be noted that the implementations are geometry-specific due to the functional form of the spatial distribution and that different basis functions could be chosen for a given geometry. The implementations described in this section are meant to serve as sample formulations to illustrate the use of integral analysis techniques in Modelica models and should not be considered universal, *de facto* implementations.

2.1 Planar Geometry

As mentioned previously, integral analysis formulations are most relevant for simulations where additional information regarding spatial distribution is important. Consider the schematic in Figure 1 showing a wall with planar geometry. The wall could be modeled in Modelica with the lumped parameter formulations shown in Figure 2. The two representations reflect different modeling philosophies regarding the placement of the capacitance and flow elements. Each formulation yields a lumped estimate for the temperature distribution in the wall via the mass-averaged temperature computed in the capacitance conservation of energy. Depending on the boundary conditions, geometry and properties of the wall, transient nature of the boundary conditions, and number of capacitances used, the lumped parameter formulation may give a good representation of the actual temperature distribution in the wall. In lumped parameter formulations, higher fidelity representations of the temperature distribution can be realized by networks of lumped capacitances. Rather than adding additional capacitances to provide a better representation of the spatial temperature distribution, an integral analysis formulation can be used. This section gives an overview of the derivation of an integral analysis formulation for planar geometry.

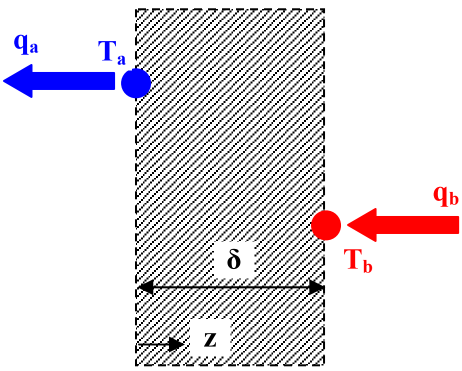
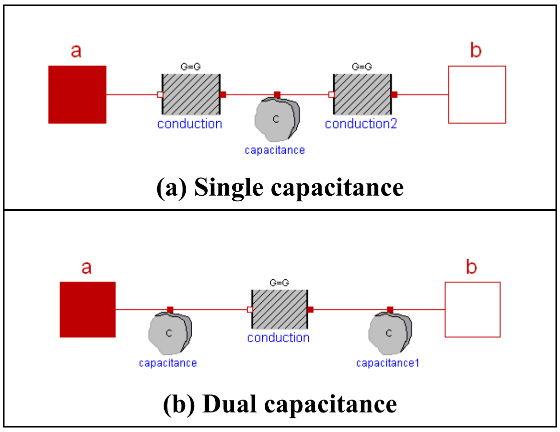


Figure 1. Planar geometry schematic



(a) Single capacitance

(b) Dual capacitance

Figure 2. Lumped formulations, planar wall

Again consider the geometry in Figure 1. The first step in the derivation is to assume the form of the temperature profile. Assuming the distribution is one dimensional in the z direction, consider the following distribution:

$$T(z,t) = T_{ss}(z,t) + T_1(z,t) \tag{1}$$

where T_{ss} is the steady-state temperature distribution for a conductive planar wall and T_1 is some assumed temperature deviation:

$$T_{ss}(z,t) = T_a(t) + \frac{z}{\delta(t)}\left[T_b(t) - T_a(t)\right] \tag{2}$$

$$T_1(z,t) = a_0(t) + a_1(t)z + a_2(t)z^2 + a_3(t)z^3 \tag{3}$$

Note that a polynomial form has been assumed for the temperature deviation but that other forms are possible.

The next step in the derivation is to determine the unknown coefficients in the temperature profile in terms of the appropriate boundary conditions. Applying the temperature and heat flow boundary conditions at z=0 and z=δ(t) and using the properties of the steady-state solution yields:

$$T_1(z,t) = \frac{q_a(t) - q_b(t)}{kA}\left(-\frac{z^2}{2\delta(t)} + \frac{z^3}{\delta(t)^2}\right) \tag{4}$$

Consistent with the initial construction of the temperature distribution, there is no contribution from the T_1 term at steady state (*i.e.* when q_a=q_b).

Though the derivation is in terms of the boundary temperatures, consider a typical interface problem where one of the boundary temperatures is unknown. By combining the integral formulation above with an overall energy balance for the volume, the boundary temperature can be determined in addition to the mean temperature. The overall energy balance for the volume based on the mass-averaged mean temperature T_m yields:

$$\frac{dU}{dt} = q_b(t) - q_a(t) \tag{5}$$

where

$$U = mc_v T_m \tag{6}$$

An equation for T_m can be derived from the definition of a mass-averaged temperature:

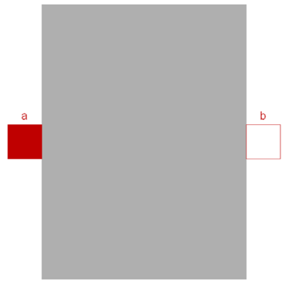
$$\rho A \delta(t) T_m(t) = \rho A \int_0^{\delta} T(z,t) dz \tag{7}$$

Using the assumed temperature distribution and performing the integration leads to the following equation:

$$T_m(t) = \frac{T_a(t) + T_b(t)}{2} + \frac{q_a(t) - q_b(t)}{kA} \frac{\delta(t)}{12} \tag{8}$$

The first term in the equation above is the mean temperature from the steady-state profile while the second term is the transient deviation from steady-state. Note that the deviation term contributes only in non-steady situations and becomes more important when the thickness of the volume increases and the thermal conductivity and surface area decrease, essentially the conditions which contribute to a measurable temperature gradient across the wall.

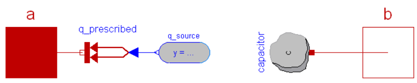
Figure 3 shows a Modelica implementation of a planar volume based on the integral analysis derivation presented above. The model uses the standard thermal connectors from the Modelica `Thermal` library. The integral formulation differs somewhat from the generic `HeatCapacitor` model in the Modelica `Thermal` library in that the model is not a volume element in the standard sense. The `HeatCapacitor` model is a single port volume model that is connected to heat flow elements and provides a temperature on its lone connector from its internal conservation of energy equation. The multiport integral planar volume is a combined volume and flow element since it contains a conservation equation that determines a connector temperature similar to a volume element in addition to providing a connector heat flow like a heat flow element based on the heat conduction through the volume that follows from the assumed temperature distribution. A conceptual representation of the integral analysis control volume is shown in Figure 3c to illustrate visually the directionality of this component. This schematic shows how the planar volume from the integral formulation is connected to a flow element on one side (connector b) and a capacitance element on the other (connector a). Because of its directional nature, it is important to connect the integral component carefully to surrounding components to ensure a consistent, complete model.



(a) Diagram

```
protected
  Modelica.SIunits.Temperature Tm "mean volume temperature";
  Modelica.SIunits.Temperature Tm_ss "steady state mean  temperature";
  Modelica.SIunits.Temperature Tm_1 "non-steady state mean  temperature
  Modelica.SIunits.HeatFlowRate q_cond "conduction through volume";
  Modelica.SIunits.MassFlowRate mdot "mass flow rate into volume";
  Modelica.SIunits.SpecificInternalEnergy U "internal energy of volume"
initial equation
  U = mass*props.cp*Tinit;
equation
  delta = mass/(props.rho*A);
  q_cond = props.k*A*(b.T - a.T)/delta;
  U = mass*props.cp*Tm;
  der(U) = b.Q_dot - q_cond + mdot*props.cp*Tm;
  mdot = der(mass);
  Tm_ss = 0.5*(a.T + b.T);
  Tm_1 = (a.Q_dot + b.Q_dot)/(props.k*A)*delta/12;
  Tm = Tm_ss + Tm_1;
  a.Q_dot = -q_cond;
```

(b) Code excerpt



(c) Conceptual representation

Figure 3. Modelica implementation of planar volume with integral analysis formulation

2.2 Cylindrical Geometry

The general approach used in the previous section can be applied to other geometries given appropriate choices for the temperature distributions. For cylindrical geometry with a one-dimensional temperature distribution in the radial direction, assume the following temperature distribution:

$$T(r,t) = T_{ss}(r,t) + T_1(r,t) \tag{9}$$

where the steady state temperature distribution is given by:

$$T_{ss}(z,t) = T_a(t) + \frac{\left[T_b(t) - T_a(t)\right]}{\ln\left(\frac{r_1}{r_2}\right)} \ln\left(\frac{r}{r_2}\right) \tag{10}$$

The choice of the deviation profile is again user and problem specific but could be assumed to have the same form as Eq. (3) in the radial direction. The final form of the integral analysis for cylindrical coordinates follows from the same process outlined for planar geometry: apply BCs to determine the coefficients in the deviation profile, use lumped conservation of energy in conjunction with mass-averaged temperature distribution, *etc*. The details of the derivation are omitted as they are similar to that in the planar analysis but with some slightly messier algebra due to the radial geometry.

2.3 Comments

The integral analysis formulation results in an approximate method for solution of the geometry-specific PDEs. Integral conservation of energy is maintained as in the lumped parameter formulation. However, some pieces of information used in the solution of the original PDEs are no longer applied, such as the slope boundary conditions at the interfaces, since the temperature distribution is assumed. While this method allows the modeler additional flexibility in terms of the temperature distributions and the specifics of the applications of the integral analysis principles, some care is required to ensure that the physics of the problem are consistent with the assumed distributions and the resulting formulation. The assumption of a temperature distribution throughout the layer leads to some practical limitations on model usage. For example, simulations dominated by an evolving thermal penetration depth would require reformulation since the temperature distribution does not extend through the thickness of the material and thus would not satisfy the assumed temperature distribution. The thermal penetration depth δ_t scales based on the following equation:

$$\delta_t \sim \sqrt{\alpha t} \tag{11}$$

where α is the thermal diffusivity of the material. Setting $\delta_t=\delta$ yields a relationship between the geometry, material properties, and simulation time scale from which the suitability of an integral analysis formulation can be evaluated. In general, the integral analysis formulation becomes increasingly applicable as the material thickness decreases, thermal diffusivity increases, and relevant time scale over which the boundary conditions change increases relative to the penetration depth time scale.

3 Simulation Results

Having developed some sample integral analysis formulations, this section provides some numerical examples to exercise the formulations. All simulations are performed with Dymola [10].

3.1 Planar Wall

Consider the simple test shown in Figure 4 for a planar wall of constant thickness. The wall is subjected to a constant temperature on one side and a constant heat flow on the other side. This test, while extremely simple, provides a nice example to illustrate the utility of the integral analysis formulation. Figure 5 shows the mean and boundary temperatures from simulations of a constant thickness wall with properties of iron and stainless steel [6] at a fixed boundary temperature of 293K. Note that the temperatures in the iron simulation are only slightly higher than the prescribed wall temperature due to the high thermal conductivity of iron. Since the thermal conductivity of stainless steel is about 1/5th that of iron, there is a larger temperature difference across the wall. In addition, the iron wall reaches steady state much more quickly than the stainless steel wall. While the deviation between the mean and boundary temperatures is modest in these sample simulations, the boundary temperature becomes increasingly elevated relative to the mean temperature as the material becomes less conductive. To accurately resolve these potentially-large temperature differences across the wall with a lumped parameter formulation, a network of lumped volumes would be required. Similar behavior is achieved with only a single capacitance using the integral analysis formulation. While this simple example is interesting, applications where the heat and/or mass flow are sensitive to the boundary temperature showcase more clearly the utility of the integral analysis formulation and will be presented in the next sections.

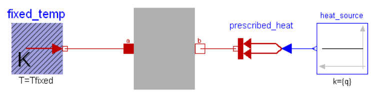


Figure 4. Planar wall, fixed heat flow and temperature boundary conditions

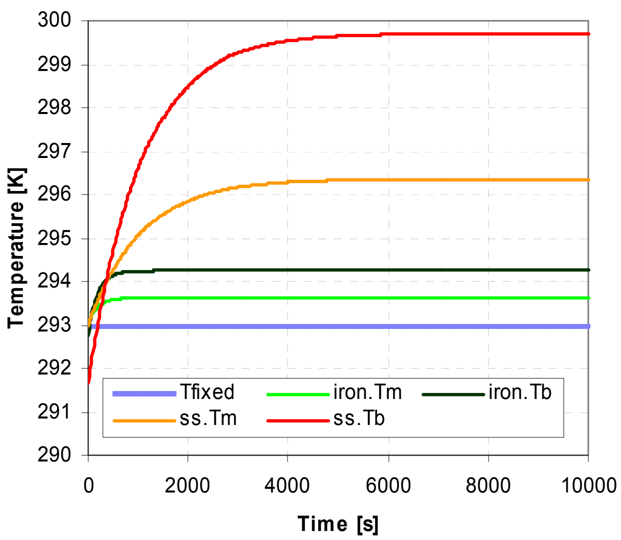


Figure 5. Simulation results, iron and stainless steel

3.2 Planar Wall with Convection

Figure 6 is a simple test similar to that in Figure 4 but with convection heat transfer calculated from the wall boundary temperature. The planar wall, modeled as stainless steel [6], is again subjected to a fixed temperature on one side. The other side is exposed to airflow at a constant velocity with a dynamic temperature given by the `ExpSine` component in the Modelica `Blocks` library [1].

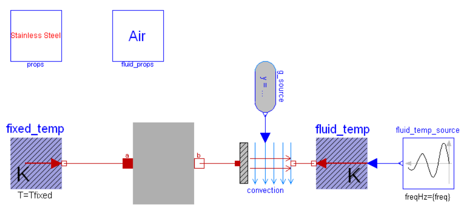


Figure 6. Planar wall with transient convection

Figure 7-Figure 8 show results from the transient convection simulations with varying frequency for the prescribed fluid temperature fluctuations, 0.001 and 0.01 Hz respectively. The top plot in each figure shows the input fluid temperature, and the bottom plot gives the fixed, mean, and interface metal temperatures from the integral analysis. As the wall is heated by the warmer fluid, a temperature gradient is again established across the wall. Unlike the fixed heat flow simulations in the previous section, the convective heat flow boundary condition is calculated from the interface temperature and, along with the fluctuating fluid temperature, adds additional transient dynamics. It is interesting to note the way in which the fluid temperature fluctuations are reflected in the mean and interface temperatures. While the mean temperature also exhibits some characteristics of the input temperature oscillations, they are damped out by the capacitance of the wall. The interface temperature, however, is significantly more oscillatory, as is to be expected. As the frequency of the oscillations increases in Figure 8, the mean temperature hardly reflects any of the oscillations despite the high frequency oscillations in the interface temperature. By introducing some notion of the temperature distribution within the volume, the integral analysis formulation provides a mechanism for a higher fidelity representation of both the spatial distribution in the volume (*i.e.* the difference between the mean and interface temperatures) and the differences in transient response (*i.e.* fast response at the interface and damped response in the mean).

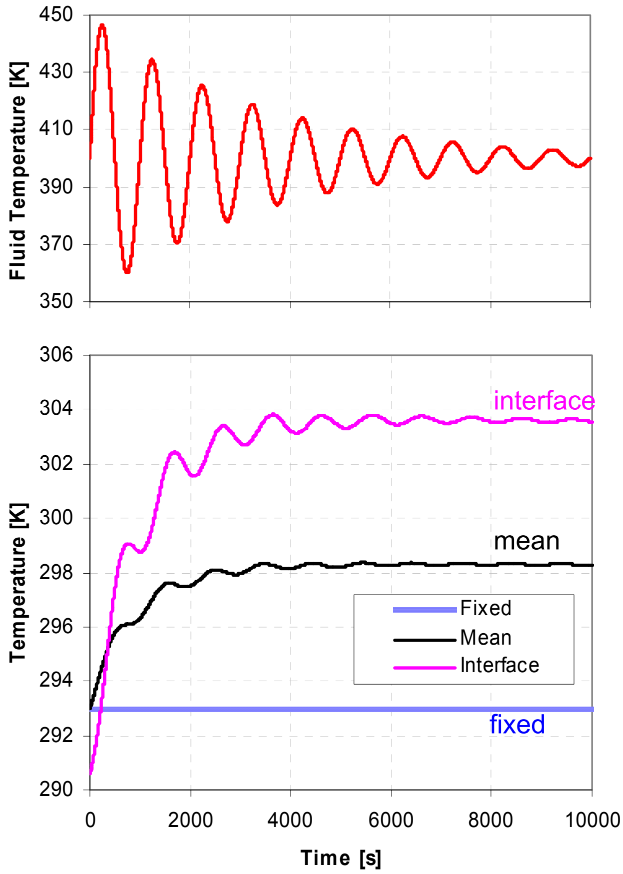


Figure 7. Simulation results, frequency=0.001Hz

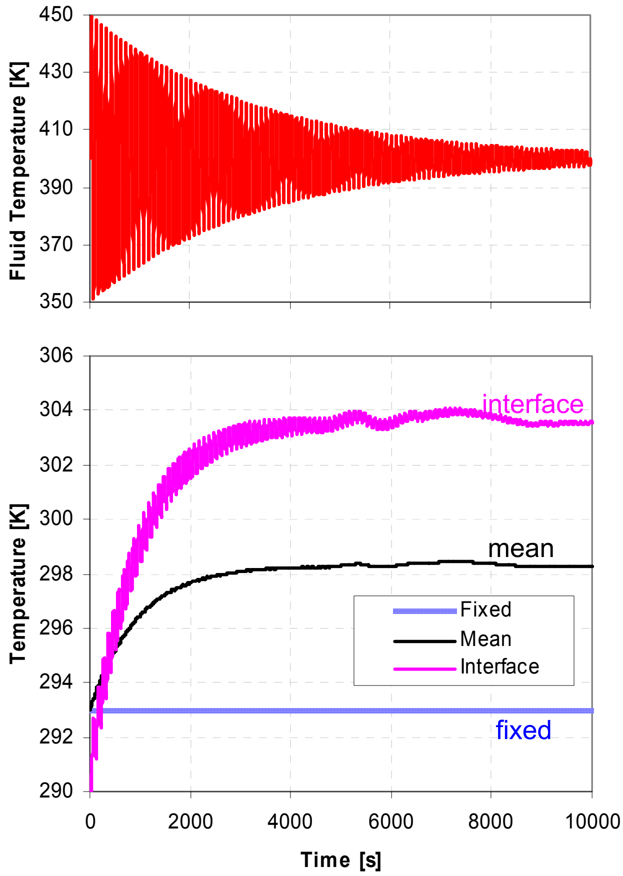


Figure 8. Simulation results, frequency=0.01Hz

3.3 Simulation with Mass/Heat Transfer

While the previous examples contained only heat transfer physics for a layer of constant thickness, the original derivation allowed for dynamic geometry resulting from heat and mass transfer. The example in this section simulates the fouling layer build-up and subsequent thermal degradation common in industrial heat exchangers. Since the fouling caused by deposition of particulates and condensation of vapor phase materials is highly-sensitive to the interface temperature between the fouling layer and the gas [11], an integral analysis formulation is used to represent the dynamics of the fouling layer.

Figure 9 shows a simple test model for simulating the effects of a deposition layer in a pipe. The inner pipe wall is assumed to be at a constant temperature, and the deposition layer is modeled using the cylindrical integral analysis formulation outlined in Section 2.2. The model consists of standard convective heat transfer based on the Sieder-Tate Nusselt number correlation for pipes [6] and a boundary layer formulation for thermally-induced particulate mass transfer [12]. Material properties for air are used for the flowing medium in the pipe, and the deposition layer is assumed to have the material properties of asphalt [6].

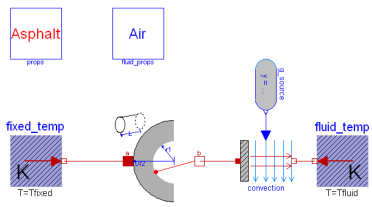


Figure 9. Pipe deposition layer with heat and mass transfer

Figure 10 shows simulation results for the pipe deposition model. The model was simulated with a fixed mass flow rate and inlet gas temperature. The simulations show the slow degradation in heat transfer performance as the deposition layer grows, thus providing an additional thermal resistance between the hot gas and the cool pipe wall. This degradation is evidenced by the increasing gas exit temperatures and alternatively by the decreasing effectiveness ε, defined in the following way for constant mass flow conditions:

$$\varepsilon = \frac{T_{gas,in} - T_{gas,out}}{T_{gas,in} - T_{wall}} \qquad (12)$$

Note the difference between the mean layer temperature and the interface temperature. Since the flowing medium interacts with the layer at the interface temperature for both the heat and mass transfer dynamics, it is important to capture this elevated interface temperature relative to the mean. Furthermore, since the elevated interface temperature and subsequent thermal degradation result from the dynamic layer thickness, it is also important to capture the transient nature of the layer growth. The integral analysis formulation allows a higher fidelity representation of the spatial temperature distribution in the layer without the need for a network of heat transfer components to represent the layer.

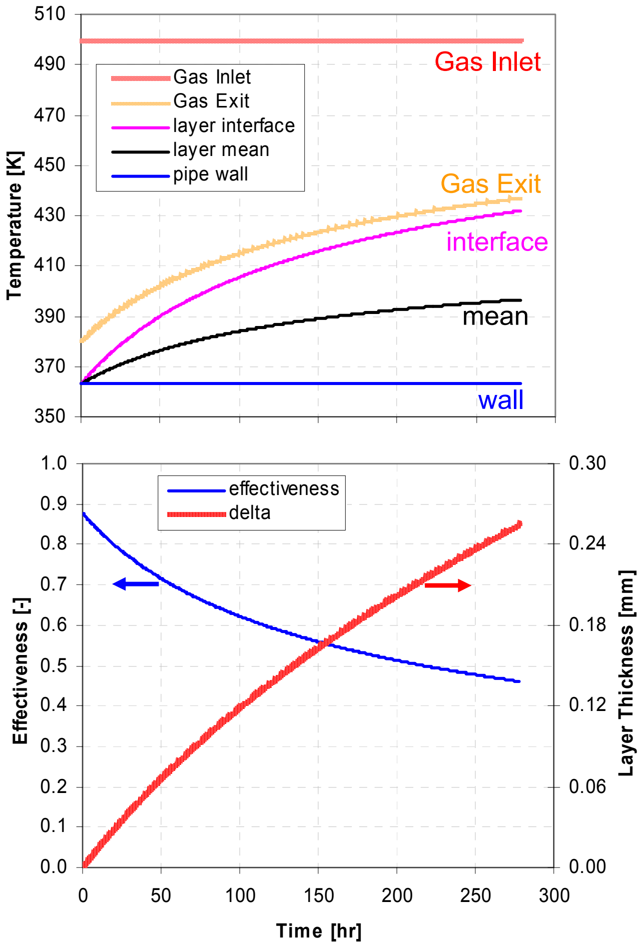


Figure 10. Pipe deposition simulation results

4 Conclusions

This paper illustrates an extension of the application of the Modelica language to thermo-fluid problems using an integral analysis approach. The sample formulations presented here give details regarding the development and implementation of the integral analysis approach in Modelica for different geometries. This approach allows the computational benefits of a lumped parameter formulation with additional details regarding the temperature distribution across the volume. In particular, the integral analysis formulation is especially useful for problems with interface dynamics, particularly those which require accurate resolution of the interface conditions to obtain the appropriate dynamic physical response.

Acknowledgements

The author gratefully acknowledges Chuck Newman for his valuable discussions regarding this work.

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