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Abstract

In this report we discuss object-oriented approaches to modelling of process systems. In particular we focus on the problem of describing flow properties such as temperature and concentrations. The basic problem is that the causality depends on the flow direction. If we have a flow from a tank A to a tank B the temperature of the flow depends on the temperature in tank A. On the other hand if the flow goes from B to A the flow temperature depends on the temperature in tank B. In the object-oriented approach we would like to encapsulate the behaviour descriptions in model components. In this report we discuss some approaches to handle this. Another problem is that the behaviour of some components, like valves and pumps, is independent of many of the flow properties. Thus it is of interest to provide model components that can handle flow descriptions of different complexity automatically. Some of the ideas presented in the report are implemented in Omola and have been used for simulation in OmSim.

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Object-Oriented Modelling of Flows in Process Systems

1. Introduction

In process systems it is usual to deal with the properties of fluids. As a simple, but illustrative example, consider a system composed with two coupled tanks (Figure 1). The model of that system should provide the equations describing the temperature of the fluid in the two tanks. The evolution of the temperatures in each tank will depend on whether the flow between the two tanks goes from *Tank A* to *Tank B* or viceversa. Assume, as indicated in Figure 1, that the flow is positive if it goes from *Tank A* to *Tank B* and negative otherwise. The heat balances for the two tanks are:

$$\begin{aligned} \tfrac{d}{dt}(\rho V_a c T_a) &= -\rho c T Q \\ \tfrac{d}{dt}(\rho V_b c T_b) &= \rho c T Q \end{aligned} \tag{1}$$

and the temperature T of the flow between both tanks is:

$$T = \text{If} \quad Q > 0 \quad \text{Then} \quad T_a \quad \text{Else} \quad T_b \tag{2}$$

As seen, it is not difficult to develop a model describing the behaviour of the total system. But since a modular approach is desired, some questions can be made about how to model each of the elements of the system. So that a model for the system can be described by putting together model components like tanks, pipelines, valves and pumps.

The Equation 2 implies that the causality in the system depends on the direction of the flow. When developing basic model components it is easy to see that Equation 1 which describes the heat balance of a tank should be included in the tank model. But where should Equation 2 be put? This equation refers to the temperature of both tanks and of the flow. In a modular approach it is, at least, rather undesirable to include equations in a module which refers to others modules, thus an equation inside a tank can not explicitly refer to the temperature of the fluid at other element. Moreover, it can not be used the same type models for the two tanks since that would imply that we get Equation 2 twice.

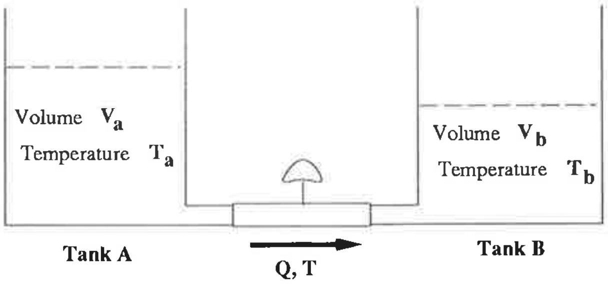

Figure 1. Two coupled Tanks

The aim of this work to discuss the problems and possible modelling solutions of describing in a modular way the elements which compose a process system and their interactions.

2. Modelling a Process System

The main objective should be to provide the user with nice descriptions of the different elements which compose a process system. So it should be easy for the user to describe the system by the putting together such model elements [Nilsson, 1993].

A model provides a description of a physical element. The model describes the behaviour of the element and its interactions with other elements. Within the context of both structured modelling languages and object oriented modelling languages, the interface of the model to describe interaction with its environment is defined by the meanings of so-called *Cuts* or *Terminals*, whereas the behavior of the element represented in the model is described in the so-called *Realization*. The set of model components and the set of connections constitute the *topological model* of the system.

The physical meaning of the connections of two elements through their terminals is that the interaction between the two elements is then established. A connection between two terminals implies usually two kinds of equations which one to one relates all the variables of the two interfaces. Depending on the quantity described by the variable, it can be distinguished two differents equations: the so-called *across* variables define equality equations; the so-called *through* or *flow* variables define 'sum to zero' equations [Cellier, 1991].

Process and Transport elements

In this work we focus on the problem of how to model the different elements which compose a system and how to describe their interfaces. A possible approach, when modelling process systems, is to distinguish between those elements which are capables of storing fluid and transforming its properties (heat, mix, chemical reactions, etc), we call them *Process Elements*, and those ones which merely acts as transport elements and links the formers (pipes, pumps, valves, etc).

The model of a process element should describe the dynamics of the properties of the fluid like the amount of mass stored, the temperature of the fluid and so on. Important attributes when modelling transport elements are pressure drop ΔP and mass flow rate Q. Often, a static non-linear relation used to relate these two properties in a duct is:

$$\Delta P = \frac{\rho}{C_v^2}|Q|Q \tag{3}$$

Therefore, a model which describes a physical duct will need both information about the mathematical expressions for the physics relations cause→effect (a nonzero pressure's drop implies a flow), and about the dimensional characteristics of the duct and also about the properties of the fluid (density, viscosity, etc).

A possible graphical description of the model of a duct is shown at Figure 2. The behaviour description relates mass flow rate and pressure drop. To describe the interaction between the duct and the components at each end, we would like the pressures to be equal and the flows sum to zero. It is thus useful to introduce at the terminal two kind of variables for a single physical attribute. The pressure at each end of the duct can be described by an *across* variable and the mass flow rate by a *through* variable. Therefore, when connecting one of the terminals of the duct,

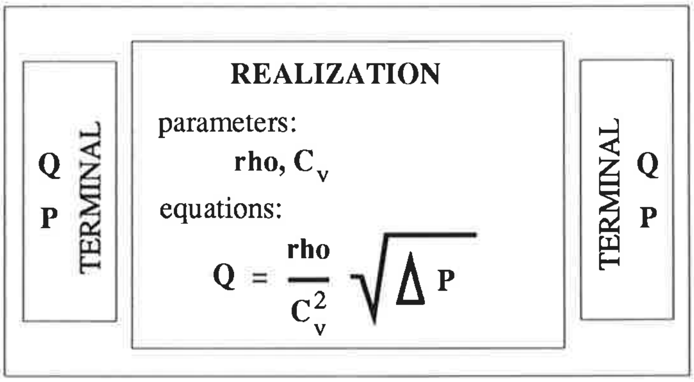

Figure 2. Structure of a model of a Duct

say A, and the terminal of other component, say B, the following equations will be established:

$$\begin{aligned} P_A &= P_B \\ Q_A + Q_B &= 0 \end{aligned}$$

What these equations are saying is: the two pressures are equal at a connection point and the sum of flows incoming at this point is zero. However, they do not say anything about other properties of the fluid.

The question now is how to include the information about other properties of the flow in the terminals and how to handle it in the different types of components. The process elements describe different thermodynamical phenomena over the fluid. Therefore such kind of components determine its properties. Transport elements describe the flow between process elements and also have to describe the transmission of the properties of the fluid flowing along them. The problem is that the causality is determined by the directions of the flows. Thus, if a new variable is included in the terminal of a component to describe, for example, the temperature of the fluid a discontinuity will be found when connecting two components since the temperature at the terminal will be the temperature of the fluid at the left component whether the flow goes from left to right or the temperature at the right component otherwise. Hence it seems necessary to have two variables for describing the temperature at a terminal, one for describing the temperature of the fluid at one side of the cut and one for the fluid at the other side. The models of the components will decide which of both variables have the correct temperature according with the direction of the flow.

Modelling the properties of the flow

In order to introduce some ideas, we will focus on the system introduced at Figure 1. Assume the dynamics of the temperature in a tank is modeled as the heat balance

$$\frac{d}{dt}(\rho V c T) = \rho c T_q Q \tag{4}$$

where T is the temperature of the fluid in the tank, T_q is the temperature of the flow, Q is the flow rate into the tank, V the volume of fluid in the tank and ρ and c are the density and the specific heat capacity of the fluid respectively.

So the information needed in order to describe the temperature inside a tank involves both the flow rate at its input-output points and the flow's temperature. The temperature of the flow T_q will be the temperature T inside the tank if the flow goes out and one of the variables describing the temperature at the terminal can be used to express this situation. A question can be made at this point: which of the two tank is determining the temperature of the flow between them?. Since the transports elements describe how the flow goes between the tanks it seems natural that such components should decide which is the temperature of the flow. Thus, the relation ***"The temperature of the flow T_q will be the temperature T at left terminal if the flow goes from left to right and just the opposite if the flow changes its direction"*** can be postulated in the models of transport elements. That can be done by the conditional relation

$$T_q = \text{if} \quad Q > 0 \quad \text{then} \quad T_{Left} \quad \text{else} \quad T_{Right} \tag{5}$$

and also the question about where to include the Equation 2 made in Section 1 is now answered.

Once the temperature of the flow T_q is known, a simple answer to the question of how to report it to the tanks is the use of the second variable describing the temperature at the terminals. Unfortunately, this solution involves complicated terminals and difficult to handle conditional structures. Other possible approaches will be discussed in later sections.

A Duct Model in Omola

Figure 3 lists an Omola [Mattsson and Andersson, 1993, Andersson *et al.*, 1994] definition of terminals implementing the requirements discussed in previous section. When a `SimpleTerminal` is connected an equality equations is generated whereas a zero sum equation is generated when connecting `Zero- SumTerminal`.

An structured terminal class `ProcessTerminal` is defined from single terminals. A connection between two record terminals implies the connection of each of their components.The terminal T_q should describe the temperature of the fluid flowing through the terminal, according with the ideas presented before, and the purpose of the terminal T is to generate the equation to set up which of the elements connected is establishing the temperature.

Conditional construct introduced in the previous section (Eq. 5), is implemented by the equation:

```
Tq = If Q>0 Then T1.T Else T2.T
```

```
PressureTerminal ISA SimpleTerminal WITH
   unit := "Pa";
   quantity := "pressure";
END;
FlowTerminal ISA ZeroSumTerminal WITH
   unit := "kg/s";
   quantity := "mass.flow.rate";
END;
TempTerminal ISA SimpleTerminal WITH
   unit := "K";
   quantity := "thermodynamic.temperature";
END;
ProcesTerminal ISA RecordTerminal WITH
   P  ISA PressureTerminal;
   Q  ISA FlowTerminal;
   T  ISA TempTerminal;
   Tq ISA TempTerminal;
END;
```

Figure 3. Terminal definition in Omola

```
Duct ISA Model WITH
%% Terminals:
    T1,T2 ISA ProcesTerminal;
%% Variables:
    P     TYPE Real;
    Q     TYPE Real;
    Tq    TYPE Real;
    alpha TYPE DISCRETE Integer;
%% Equations:
    P = T1.P - T2.P;
    T1.Q + T2.Q = 0;
    Q = T1.Q;
    T1.Tq = T2.Tq;
    T1.Tq = Tq;
    Tq = IF Q > 0 THEN T1.T ELSE T2.T;
END;
PipeLine ISA Duct WITH
%% Parameters:
    Cv, rho  ISA Parameter;
%% Equations:
    P = rho/sqr(Cv)*abs(Q)*Q;
END;
```

Figure 4. Omola models of a Duct and a Pipe

Figure 4 list the model of a duct. The model `Duct` is used as a *superclass* to define differents types of ducts as pipes, valves, etc. The model for a Pipeline derived from the class `Duct` contains the flow rate relation from equation 3. Therefore, the transport element which has been defined, will decide from which of the process elements it has to take the information about temperature and, to which has to transmit that information, depending on direction of the flow.

It is now easy to include the heat balance described by Equation 4 in a process element model. A model for a tank with constant area and four flow connections points is listed at Figure 5. The density ρ and the specific heat capacity c of the fluid are supposed to be constants.

```
Tank ISA Model WITH
%% Terminals:
    T1, T2 ISA ProcesTerminal;
%% Parameters:
    Area, rho, c, Patm, g ISA Parameter;
%% Variables:
    Vol,T,InFlow,H      TYPE Real;
%% Level:
    T1.P   = Patm;  T2.P   = sqrt(Patm+g*H);
    InFlow = T1.Q + T2.Q;
    Vol'   = InFlow;
    H      = Vol/Area;
%% Temperature:
    T1.T = T; T2.T = T;
    (Vol*rho*c*T)' = rho*c*(T1.Q*T1.Tq + T2.Q*T2.Tq);
END;
```

Figure 5. Omola model of a Tank

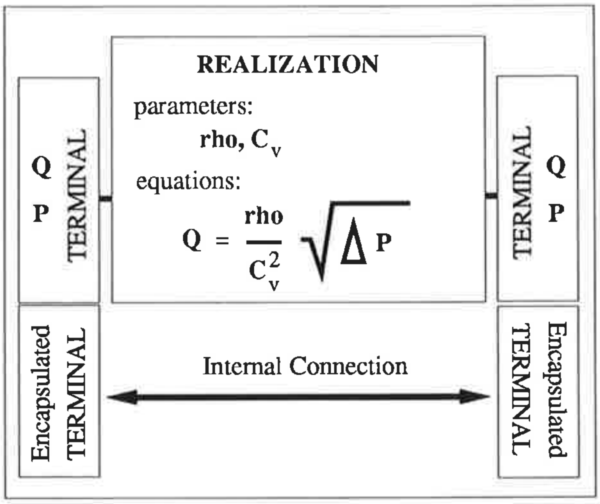

Figure 6. Encapsulated Terminals

3. Further considerations on duct's modelling

If a model of a flow includes many properties it is laborious to write down all the equations for the transmission of these properties in a transport model. A possible approach to avoid detailing how all the properties associated into the fluid are transmitted through transport elements may be defining a kind of internal connection at the element. The internal connection will describe the transmission of information in a similar way as connections of terminals do. Such connection will not reduce the number of variables at the terminal, but will make easier the model development task and simple trivial equations reduction could be made during simulation program's generation. A graphical representation of such connections is shown at Figure 6.

Since it is not longer necessary to have access in the model of the transport element to the properties of the fluid, they can be encapsulated in such way that the modeller have not to care about their meaning. Inside that internal connection a switch between the variables describing the two possibles temperatures of the fluid is done (see Fig.7). The new internal relation describe only the temperature of the two elements linked by the transport element.

So the problem of deciding which is the real temperature of the fluid is transferred to the models for process elements. These models will need some conditional structure to decide whether a fluid goes into the element or out from it. Therefore the heat balance in equation 4 has not information enough to describe the new situation, so some changes have to be made on it:

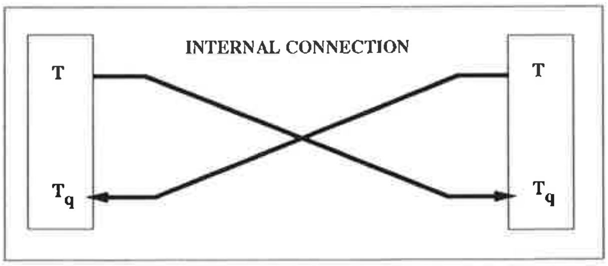

Figure 7. Graphic for a switching internal connection.

$$\frac{d}{dt}(\rho V c T) = \rho c(\alpha T + (1-\alpha)T_q)Q \tag{6}$$

$$\alpha = \quad \text{if} \quad Q > 0 \quad \text{then} \quad 0 \quad \text{else} \quad 1 \tag{7}$$

where T is the temperature inside the tank, T_q describes the temperature of the possible inflow fluid. The flow rate Q is assumed to be positive if is an inflow and negative otherwise.

In this new approach, the conditional structure (equation 7) has been transferred from the transport element model to the process element model. This is a more natural way since is the process element which has to describe the temperature's dynamics and the transport element becomes a kind of *generalized terminal*, in the sense of transmitting information. However it is still a disliked conditional description of behaviour.

Implementation in Omola of an Internal Switch Connection

Some changes have to be made on the definitions of the terminals in order to implement the idea of encapsulated terminals. The listing of new definitions is shown at Figure 8. `ProcesTerminal` is defined such way that the two variables describing the temperature of the fluid are included inside the record terminal `Temp`. It is necessary to remark that depending on the element the use of the encapsulated part of the terminal will be different. For transport elements does not matter which is the information encapsulated for making the internal connection. However, process elements will need to access to the information encapsulated.

Since at present Omola does not include a specific attribute to set up internal connections between terminals inside the element, a model has been designed in order to emulate such kind of connection. The model is listed at Figure 9 and it is its aim to include the equations needed to establish the switch inside two encapsulated terminals as was introduced at the beginning of the section (see Fig. 7).

The model for the duct will be quite simplified since it do not contains any reference to the properties of the fluid, nor about how to handle with the transmission of that information. Except, of course, for the description of internal connection. A listing of the new definition for the class `Duct` is shown at Figure 10.

The modifications introduced on definitions of terminals may cause problems to those models which access to the encapsulated part of the terminals and some little changes have to be made. This is not the case for the model `PipeLine`, which inherits all the attributes from its super class `Duct`. Model definition for pipeline does not need implicit access to terminals since it is defined on its superclass, thus no changes will be necessary.

But some modifications will be necessary on the model for the tank. As it is shown in Figure 11, the conditional construct at equation 7 has been implemented as manipulation of state events [Andersson, 1993]. When the flow `T2.Q` is positive

```
TemperatureTerminal ISA RecordTerminal WITH
   T, Tq  ISA TempTerminal;
END;
ProcesTerminal ISA RecordTerminal WITH
   P    ISA PressureTerminal;
   Q    ISA FlowTerminal;
   Temp ISA TemperatureTerminal;
END;
```

Figure 8. Encapsulated Terminals

```
SwitchTerminal ISA Model WITH
    C1, C2 ISA TemperatureTerminal;
    C1.Tq = C2.T;
    C2.Tq = C1.T;
END;
```

Figure 9. Emulation for an Internal Switch Connection.

```
Duct ISA Model WITH
%%  Terminals:
    T1, T2 ISA ProcesTerminal;
%%  Parameter:
    Length ISA Parameter;
%%  Internal connection:
    Switch ISA SwitchTerminal;
    T1.Temp AT Switch.C1;
    T2.Temp AT Switch.C2;
%%  Parameter propagation:
    Switch.Length := Length;
%%  Variables:
    P,Q     TYPE Real;
%%  Equations:
    T1.Q + T2.Q = 0;
    P = T1.P - T2.P;
    Q = T1.Q;
END;
```

Figure 10. Class definition for a Duct including Internal Switch Connection

the associated variable **alpha** take value 0 and 1 when is outflowing. Detailed access to encapsulated terminal is needed to report the environment the temperature of the fluid inside the tank, and to receive from the environment the incoming flow's temperature when necessary.

```
Tank ISA Model WITH
%%  Terminals:
    T1, T2 ISA ProcesTerminal;
%%  Parameters:
    Area, rho, c, Patm, g ISA Parameter;
%%  Variables:
    Vol,T,InFlow,H  TYPE Real;
    alpha           TYPE DISCRETE Integer;
%%  Level:
    T1.P   = Patm;  T2.P   = sqrt(Patm+g*H);
    InFlow = T1.Q + T2.Q;
    Vol'   = InFlow;
    H      = Vol/Area;
%%  Temperature:
    T1.Temp.T = T; T2.Temp.T = T;
    (Vol*rho*c*T)' = rho*c*(T1.Q*T1.Temp.Tq +
                        + T2.Q*(alpha*T + (1-alpha)*T2.Temp.Tq);
    alpha = IF T2.Q > 0 THEN 0 ELSE 1;
END;
```

Figure 11. New Model for a two inlets Tank

4. Physical causality

The two previous approaches are based on the assumption that the causality can only be established through the connections of two components. The physical causality, when considering properties like temperature or concentration, is determined by the process elements. In order to establish the interactions between two process elements is necessary to carry on all the information related to these properties through the transport elements [M.A. Piera, 1993]. As seen in the previous sections, this requirement implies extra work when modelling transport elements to be able to establish physical interactions between components which are not directly connected.

Consider again the system in Figure 1. When the model for the tank is being developed the only thing that can be assured about Equation 4 is that, if the fluid goes out from the tank, its temperature T_q will be the temperature T inside the tank. Therefore, the physical causality is partially established since only one of the possibilities has been contemplated.

In order to complete the causality on the temperature of the flow it should be possible to analyse the flow path and find other process elements which are determining the properties of the flow in the case when the direction is into the tank. In other words, it should be possible to analyse the differents interactions between components not only considering the couples of interconnected components but also the ***physical coupling*** which appears in the whole system and which determines the physical causalities on certain properties.

A natural way of searching physical causality, since the properties are carried by the flow, is to follow the possible paths for the flow between process elements, i.e., the chains of transport elements between process elements.

Let's follow our example (the subindexes A and B are included to distinguish the equations of the two tanks). The temperature in tank A will be described by the heat balance

$$\frac{d}{dt}(\rho V_A c T_A) = \rho c T_a Q_a$$

and the causality on the outflow by the conditional equation

$$\text{If} \quad Q_a > 0 \quad \text{Then} \quad T_a := T_A$$

Analogously, the same equations are established in tank B

$$\frac{d}{dt}(\rho V_B c T_B) = \rho c T_b Q_b$$

and the causality on the outflow by the conditional equation

$$\text{If} \quad Q_b > 0 \quad \text{Then} \quad T_b := T_B$$

One thing is left. It should be found that the flow between the two tanks and its temperature T_q are uniques and always $Q_a = -Q_b$. Hence, the following conditional equation could be postulated

$$\text{If} \quad Q_A > 0 \quad \text{Then} \quad T_q := T_A \quad \text{Else} \quad T_q := T_B \tag{8}$$

Consequently T_q refers to the same property and the physical causality on the temperature of the flow is then completed. Is a simple matter of analysing the transport element to find such relation. As can be seen analysing Figure 12, the result $Q_a = -Q_b$ can be deduced from the equations generated when connecting the three components

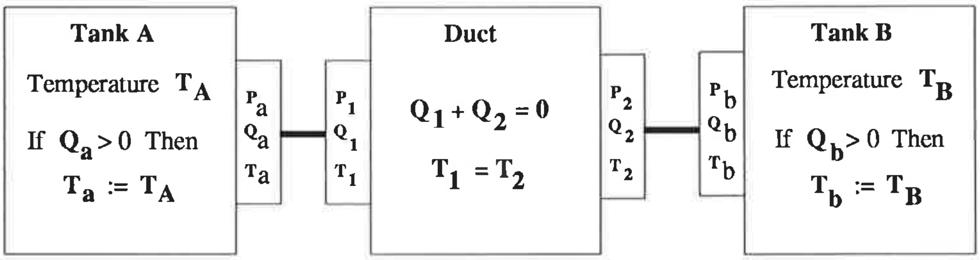

Figure 12. Graphical description of the interesting equations when searching physical causality

$$Q_a + Q_1 = 0$$
$$Q_b + Q_2 = 0$$

and from the duct realization

$$Q_1 + Q_2 = 0$$

Therefore, it is possible to say that conditions $Q_a > 0$ and $Q_b > 0$ are complementaries. Now, to complete the equation, it can be deduced from all the equalitys generated for the across variables T_i that the temperature of the flow T_q is unique, so that Equation8 can be postulated (notice the analogy to Equation 2).

As seen, if this automated procedure is supplied by the modelling tool, the task of developing models when considering the transmission of properties of a flow is significantly simplified.

5. Conclusions

The problems when modelling the transmission of properties of a fluid in a process system have been presented and two different approaches introduced.

First, has been shown that one possible solution is to introduce one terminal component to describe the properties on the "left" side of the cut and one more terminal component for the "right" side. As a consequence, it has to be remarked that complicated terminals are defined because duplicate variables for describing a single property is needed, and the difficulty of handling with conditional structures to transmit the information.

A first solution drove to complex models for transport elements when defining conditional equations inside the model for transmitting information. Additionally, an objection could be made about the necessity of defining equations in a model involving information which is not implicitly used in model. Thus, in the model development phase for a duct, a large number of things not belonging to its hydrodynamics behavior have to be considered. And that is not desirable. Furthermore, the number of equations and the complexity of its analysis is increased for the single reason of transmitting information. Despite the complexity of developing model for transport elements, it may be considered that a model developer will probably make more models for process elements.

In order to avoid complicated models of transport elements, a second possible solution is adopted by defining internal switch connections. But, no more than one model enclosing internal switch connection can be connected. Otherwise it is not very clear which of the switching variables at the terminal will contain the desired value. Sometimes is also necessary to know the magnitudes of some properties whose describing variables have been encapsulated. For example when the density of the fluid is not constant. Therefore that information should not be encapsulated. However, it has to be remarked that the complexity of the model of transport elements is not increased when the number of attributes to be transmitted increases.

These two solutions are based on the assumption that the interactions between two components can be established only through its connection. But the physical causality over some properties of a system can be established by components which are not directly connected. In a second approach it is assumed that the modelling tool is able to supply a physical causality analysis to find such kind of interactions. Hence, the model developing task and the models themselves are quite simplified.

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