ON PROCESS MODELLING USING PHYSICAL ORIENTED AND PHENOMENA BASED PRINCIPLES

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Abstract: This work presents a modelling framework based on phenomena description of the process. The approach is taken to easy understand and construct process model in heterogeneous possible distributed modelling and simulation environments. A simplified case study of a heat exchanger is considered and Modelica modelling language to check the proposed concept. The partial results are promising and the research effort will be extended in a computer aided modelling environment based on phenomena.

Keywords: Modelling, Models, Behaviour, Object Modelling Techniques, Methodology, Simulation, Physical model.

1. INTRODUCTION

The decomposition of the physical plant and processes into individual objects is a powerful technique to manage complexity. The generic example is the effort under Modelica modelling language development, (Elmqvist, *et al*, 1998). The phenomena based principle supposes to use physical phenomena to describe the process under study. It is a reality that modellers must be very creative and also experts in the process studied. Another reality is that knowledge about the process, and why not about the modelling process himself, is not always re-used. The paper proposes a new way to think and to model, based on physical and phenomenological principles.

The physical orientation in modelling is not a new trend. It is used in some modelling and representations languages, (Mattson, *et al*, 1998), and it is the subject of intensive research efforts as described, for example, in (Mosterman and Biswas, 1999), (Mosterman, *et al*, 1998a, 1998b), (Cellier, *et al*, 1995). The proposed approach is a combination of physical and phenomena principles in order to improve the understandability and manageability of process models. As a case study is used a heat-exchanger. It is not the purpose to obtain a complete model to be used in control and behaviour models. It is only to show the frame-work. A more complete behaviour model can be obtained because the framework can be reused, this time like a more convenient start point, to improve (refine) the obtained models.

Object-oriented modelling of physical systems is an important research direction. The different proposals

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appearing in the literature have the following fixed points in common:

- modelling of the interaction of modules with the exterior is by ports or terminals through which energy/matter is exchanged;
- object behaviour is described in a non-causal form (i.e. without any presumption of causality among variables), typically through an implicit DAE (differential algebraic equations) system;
- events may be generated within a component model, or may come from outside the module, and may propagate through modules.

Details can be found in (Borutzky, 1996), (Rames, *et al*, 1998). In some modelling and simulation environments based on objects, in order to reduce the index of the equation system that must be solved for example, it is possible to have different (some of them wrong) physical causality of the models. In this sense, the modeller must be quite careful, in order to solve a contradiction in obtaining:

- an *a-causal* model, to respect the general principle of physical object-oriented paradigm, that means to not impose any causality;
- a real-compliant model, in the sense to have a model with the same behaviour like the real modelled process.

Unfortunately, a general answer and solution cannot be done, and the right causality must be checked for every sub-model. Any changed causality restricts the generality of the model an must be written some how, some where, explicitly by remarks or comments.

As case study a heat-exchanger is used as a complex multi-scale and multi-domain phenomena. Two models are considered and described in the following. One is classic based on equations, and used here as reference, and the other one is based on phenomena. The main assumption to simplify the process are: (A1) - a single medium liquid flows: hot water and cold water, and (A2) - the physical dimension of the plant are small, that means it is not the objective into modelling pressure, temperature or velocity profiles over holes or pipes (ducts) ends. The heat exchanger is considered designed from two ducts and a wall for interface. The connections among sub-models are presented in Fig. 1. The behaviour models based on equations is well studied. Some good references are (Granet, 1980), (Tominaga and Tamaki, 1997) and (Tiller, 2000). The pressure drop over the duct is modelled as:

$$p_1 - p_2 = \frac{?}{C_v^2} \cdot |q_{12}| \cdot q_{12} \qquad (1)$$

where p_1 and p_2 are the pressures at the two ports, q_{12} is the volume flow rate from port 1 to port 2, ρ is the density of the fluid and C_v is a constant. This can be interpreted as a functional equation for the duct. The mass balance for the duct is:

$$q_1 = q_2 \qquad (2)$$

that means the *volume flow rate* is the same at the input and at the output of the heat exchanger. The heat balance of a duct gives

$$\frac{d}{dt}(?VcT) = ?c(T_1 - T_2) \cdot q_{12} + F \qquad (3)$$

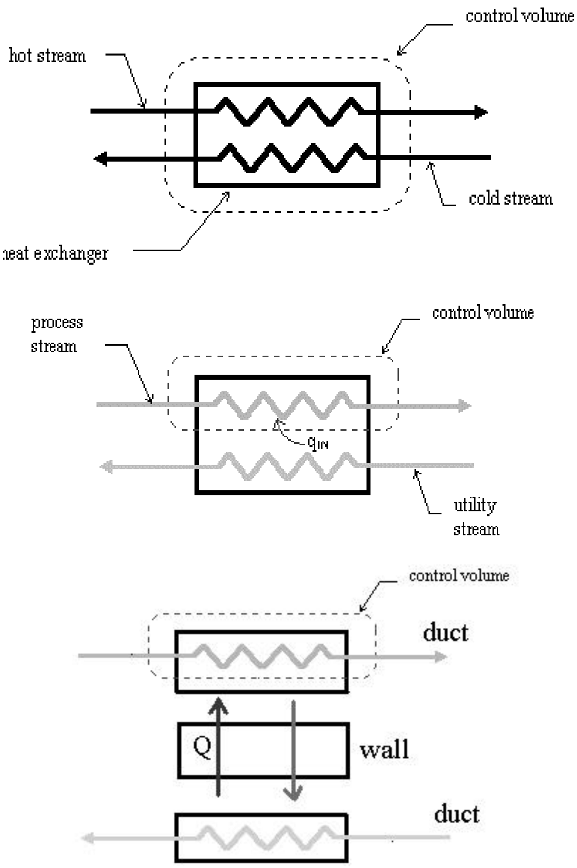

Fig. 1. Steps decomposition of the physical heat exchanger into physical sub-models

where T_1 and T_2 are the temperatures at the two ports, T is a representative mean temperature of the fluid, c is the *specific heat capacity of the fluid*, V is the volume of the fluid and Φ is the rate of the heat flow across the wall into the duct. The temperature at the outlet will be assumed to be T:

$$If \quad q_{12} > 0 \quad then\ T = T_2 \quad else \quad T = T_1 \qquad (4)$$

2. THE EQUATIONS BASED MODEL

The heat (energy) balance and the functional equation for the wall:

$$F_A + F_B = 0; \qquad F_B = \frac{?Tm}{R} \qquad (5)$$

where R is the overall thermal resistance between the two ducts and ΔT_m is a suitable mean temperature difference between the ducts A and B across the section. To obtain a model that has a statically correct behaviour, the common approach is to take ΔT_m as the log-mean temperature difference, $\Delta Tl_{m,}$ defined as

$$? T_{lm} = \frac{?T_1 - ?T_2}{ln\left(?T_1 / ?T_2\right)} \tag{6}$$

where $DT_1 = T_{A,1} - T_{B,1}$ and $DT_2 = T_{A,2} = T_{B,2}$ are the temperature differences at the two ends of the duct; A and B are the two ducts. The thermal resistance, R, between the hot and cold side can be decomposed into four terms:

$$R = R_1 + R_w + R_2 + R_f \tag{7}$$

where R_A and R_B are the thermal contact resistances between the liquid in the ducts and the wall, R_w is the thermal resistance of the wall, R_f is the thermal fouling resistance due to deposits and duct on the wall. The contact resistances between a liquid and the wall are modelled as:

$$R_i = \left(h_i \cdot A_w\right)^{-1}, \; i = A,B \tag{8}$$

$$h_i = h_0 \cdot \left|\frac{q_i}{q_0}\right|^{nh} \cdot \left[1 + a_h\left(T_i - T_0\right)\right], \quad i = A,B \tag{9}$$

where h_i is the surface coefficient of heat transfer, A_w is the area of the common wall between the ducts, and h_0, n_h, q_h, and a_h are constants to be identified from measured data and T_0 is an estimation of the mean value of lowest and highest appearing temperatures. The thermal resistance of the wall, R_w, is calculated as

$$R_W = \frac{d_W}{?_W Y_W A_W} \tag{10}$$

where d_w is the thickness of the wall, λ_w is the *thermal conductivity of the wall material* and Y_w is a correction factor for the corrugation of the wall. The model of the wall needs *flow rates* and *temperatures from the models of two ducts* and the models of the ducts refers to the heat flow.

3. THE PHENOMENA BASED MODEL

Started from reality that is difficult to consider all phenomena from the real processes, the considered phenomena are divided (classified) in two categories: important, relevant or considered; un-important, negligible or un-considered.

3.1. Behaviour versus phenomena

The modeller defines the two categories in "collaboration" with the computer (which assist the modeller), which means there is a cooperative work. Both categories are made in a declarative way and finally two sets of phenomena will result. It seams to be important here to have ontology related to phenomena. The declaration and - more then that - agents of the modelling environment assist the management of such declarations. In fact, in the first step we have a mixed declaration: phenomena plus behaviour. Ordinary people can develop this blend, behaviour plus phenomena, without specialized knowledge about the considered process. Of course, latter, in the second step, the phenomena will be separated from behaviour because:

- the main goal of any modelling activity is obtain a model with the same behaviour with the modelled process;
- not all the phenomena are relevant or are important at the same epistemological level.

This metamodel is presented in Fig.2 under a class diagram representation.

All the phenomena can be structured under some cause-effect relationships and/or under domain characterization. In Fig. 2 the phenomena are considered under effort-flow causalities like in bond-graph formalism. The first set, based on pressure and flow is for the fluid domain, the second set, based on temperature and heat is for thermal domain. So far, a third set is presented, the Set_x, to show the partiality of the metamodel.

3.2 Partial metamodels based on phenomena

In Fig. 3 a partial metamodel for thermal domain is presented. It is important to observe that there are three main basic thermal phenomena, conduction, convection and radiation. Every such phenomenon needs information from a one or more (1..*) GeometryModel, from one or more MaterialModel (1..*) and one EnvironmentModel. More, the EnvironmentModel needs one or more MaterialModel in order to have the correct behaviour. All thermal phenomena have in common: a gradient of temperature, a heat transfer, a thermal resistance and a transfer area. These are common attributes which will be defined latter in concurrency with other information from *GeometryModel* and ContextModel (not presented in Fig.3, but necessary).

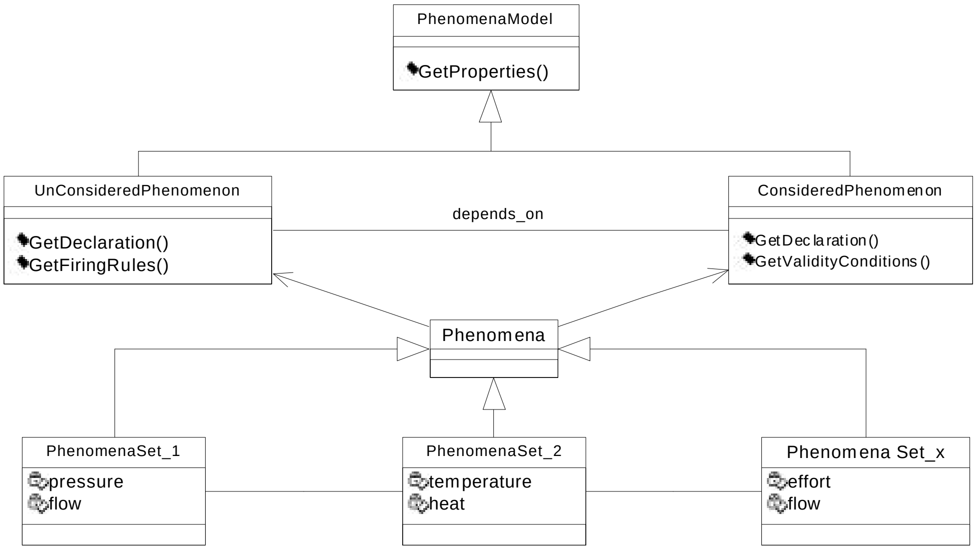

Fig. 2. The class diagram for the phenomena metamodels

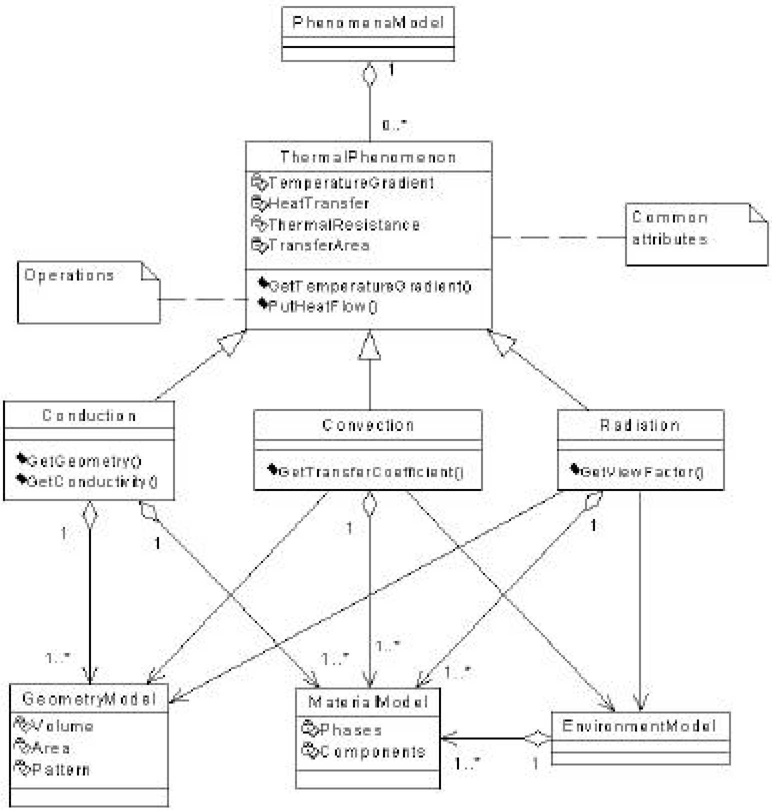

Fig. 3. A partial metamodel for thermal phenomena model in heat exchanger

The geometry model is able to send all the information from physical layer, such as volume, area, heat transfer area, and also the pattern in 3D coordination system. The *EnvironmentModel* generates all the information about the exterior of the modelled system. Mainly is based on combination of material models. Description of the phenomena use object-oriented methodology and specially by using multiple inheritance. It is possible also to use powerful techniques like class paramterization and/or redeclaration statements, like in some examples of Modelica language, (Elmqvist, *et al*, 1999).

In Fig. 4 the basic structure (composition and connections) of the duct model and wall model is presented. The approach is into considering the framework of phenomena that take place in the considered system. Mainly here are considered two domains: hydraulic or fluid domain, and thermal domain. For every phenomenon, individually considered, no important problems are. At list at the macroscopic level, some variety of solutions can be defined when considering the interaction of phenomena from the two domains. The duct is modelled by a superposition of two domain-phenomena: thermal and hydraulic. The considered phenomena from thermal domain are related to heat transfer: conduction (*hcon*), convection (*hconv*), radiation (*hrad*). From hydraulic domain only one phenomenon is considered, fluid flow based on pressure difference. The interaction between the two domains is modelled by the model "*hmf*" (heating moving fluid).

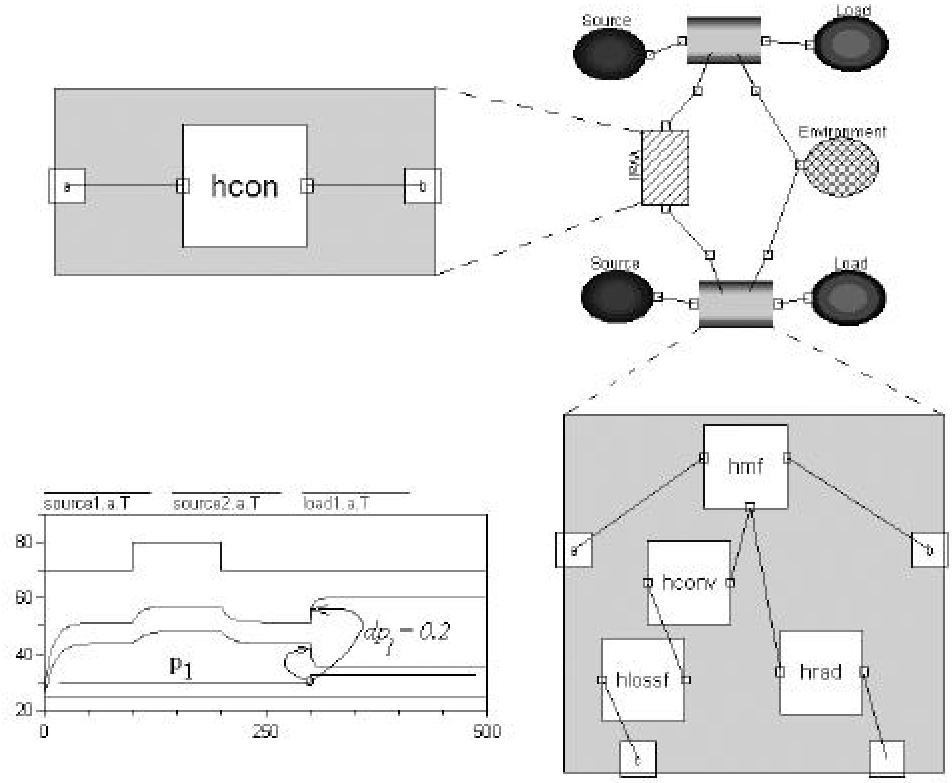

Fig. 4. Samples from a heat exchanger model based on phenomena

Another interaction phenomenon is related to heat losses by fooling, considered here in "*hlossf*" model, important to consider in the design and modelling of industrial equipments. The global behaviour of the heat exchanger is obtained by connecting phenomena. A good feature of the approach is that the sensitivity problem of models is transferred to sensitivity of phenomena. The phenomena sensitivity can be evaluated by comparing some common parameters, like thermal resistances. All the phenomena that have thermal resistances below an imposed level can be neglected.

4. SOME DETAILS OF MODELS AND SIMULATION RESULTS

The phenomena model interacts by interfaces called connectors in Modelica. For example, below it is presented the interfaces for fluid domain, for thermal domain and for thermo-fluid domain:

```
connector PortFluid "A place for stream transfer"
        Pressure p;
        flow VolFlowRate qvoldot;
end PortFluid;
connector PortHeat "A place for heat transfer"
        Temperature T;
        flow HeatFlowRate qheatdot;
end PortHeat;
connector PortThermoFluid
        extends PortFluid;
        Temperature T;
end PortThermoFluid;
```

The partial model for thermal-phenomena is:

```
partial model ThermalPhenomenon "A model for thermal domain"
        PortHeat a,b;
        Area transfer_area (min=1E-6);
        ThermalResistance Rth (min=1E-6);
        Temperature dT (start=0);
        HeatFlowRate qheatdot;
equation
        dT = a.T - b.T;
        qheatdot = qheatdot;
        a.qheatdot + b.qheatdot = 0;
end ThermalPhenomenon;
```

and a conduction phenomena is defined by

```
model HeatConduction
extends ThermalPhenomenon;
    ThermalConductivity thermalcond (start = 1);
    Thickness thick (start = 1);
Equation
    Rth = thick / thermalcond / transfer_area;
```

```
    qheatdot = dT / Rth;
end HeatConduction;
```

The final model of heat exchanger is described by:

```
model HEX "A heat exchanger"
    Duct duct1, duct2;
    Wall wall;
    HeatEnvironment henv1;
    ThermoFluidSource source1, source2;
    ThermoFluidLoad load1, load2;
equation
    connect(source1.a, duct1.a);
    connect(duct1.b, load1.a);
    connect(duct1.c, wall.a);
    connect(duct2.c, wall.b);
    connect(duct2.a, source2.a);
    connect(duct2.b, load2.a);
    connect(henv1.a, duct1.portheat_env);
    connect(henv1.a, duct2.portheat_env);
end HEX;
```

Partial simulation results are presented in Fig. 4, right side below corner. Excepting some parameters values, which are specific to geometric details and not known here, the right qualitative behaviour must be retained.

5. CONCLUSION

This work has been presented a useful framework based on phenomena to facilitate model re-use and a common level of abstraction in modelling environments. The considered approach is based on metamodels and class diagram representations of object models (phenomena) classes. In this way metamodelling can be done in a more efficient way free of context, which means without considering the geometrical details. A communication mechanism must be considered in order to cover (to adapt) the metamodels to the context when is required. By metamodelling is understood any kind of formalism to represent the knowledge concerning the construction of process models. The metamodels must be easy to understand by both computers and humans. From this point of view, a metamodel represented by class diagram and/or state (activity) transitions (in order to define then some automata) it seems to be a good way to follow. Also, the management of metamodels, history of assumptions and modifications, are important tasks to consider in the near future. The case study based on heat exchanger shows that the proposed framework is valid and can be automated under some computer aided modelling and simulation environments. The considered phenomena are from thermal domain with no reactions and phase transformations. The simulation results are very encouraging in the sense that the qualitative behaviour is correct under considered scenario. The proposed and verified modelling approach is one way to define and use a concurrent modelling architecture in complex heterogeneous and possible distributed end-users environments.

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