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Modelica Library for Hybrid Simulation of Mass Flow in Process Plants

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Abstract

Operation, control and maintenance of large process plants can be very energy and cost intensive. Optimization of the involved technical, organizational and dependent economic aspects is a non-trivial, multi-criteria problem; solving it can be supported by dynamic plant modeling.
First principles, constitutive and empirical relations are used to derive quasi-steady-state mathematical models of fluid storage and flow for a selection of physical components as are typically installed in process plants. Control logic, both on component and plant-level, is integrated using high-level hybrid language constructs of Modelica and in particular, extended Petri net formalism. The resulting Modelica library facilitates efficient composition of mass flow models of potentially large and complex plants and allows for simulative investigation of plant dynamics.

1 Introduction

Availability of process plants depends mainly on a combination of the reliability of individual installed components, the plant topology, the control system[1] and on the plant maintenance strategy and procedures. Traditional system analysis methods, as know from reliability engineering, e.g., fault tree analysis (FTA), event tree analysis (ETA), hazard and operability study (HAZOP) and failure mode and event analysis (FMEA) can lead to significant insight into the weak points of a plant with respect to performance measures as reliability, availability, safety or profitability. However, these methods lack force of expression when trying to deal with highly *dynamic systems* or systems with extensive *internal feedback loops.* Collaboration with a partner form industry–on topics of maintenance, fault detection and monitoring of process plants–has lead to the insight that performance analysis of complex process plants needs to consider not only static aspects, but also dynamic ones, not only technical, but also operational, organizational and economic factors as well.

Petri nets are well suited for modeling of discrete-event phenomena, and can be used beneficially to investigate plant availability (as demonstrated e.g., in [Fa01]), but are inherently far less convenient as a modeling formalism when confronted with physical processes exhibiting continuous-time behavior. In order to address all above mentioned aspects of process plant performance, integrated hybrid[2] dynamic modeling–unifying different formalisms–is in need.
Modelica[3], still rather new, with its multi-domain and multi-formalism modeling capabilities, seems promising in this respect. It defines a physical object-oriented modeling paradigm suitable for expressing hybrid behavior and offers respective high-level language syntax and semantic. It supports hierarchy, reuse of modeling knowledge and provides an open standard, based upon which, a couple of computer-based tools have already been created or have migrated to[4]. Several open, standard Modelica libraries exist e.g., for electric, mechanic and hydraulic systems. Among other, currently, a thermodynamics library called "Thermofluid" is being developed, see [Tu98], which could be very useful for modeling of process plants in the future as well.
In this text, primarily, mass-flow dynamics in process plants are to be investigated, and for this purpose, a new, customized library is presented. It contains models of basic equipment needed for fluid–in particular liquid–transport and storage as well as logic to control the flow of material. The library considers the flow as *quasi-steady-state*, i.e., no momentum balance is formulated; the flow is assumed to reach steady flow conditions instantly based on the current outer pressure situation and internal pressure drop characteristic.
System-level dynamics are of main interest here, not the very details of component behavior. This distinguishes it also from the available–partly commercial–hydraulics library in Dymola, which focuses on hydraulics as used in control systems. Emphasis is on

[1] Both automatic control and human operator interaction.

[2] The term "hybrid" is used here to denote combined discrete-event and continuous-time behavior.

[3] Modelica is a trademark of the Modelica Association (http://www.modelica.org

[4] In this text, the tool "Dymola" is used; Dymola is a registered trademark of Dynasim AB, Sweden, http://www.dynasim.se

ease-of-use, scalability and extendibility. Models generated with the library can be used for experimental design studies, control scheme optimization, de-bottle-necking, re-engineering of already commissioned plants. The paper first discusses basic physics and mathematics of modeling fluid flow components before addressing implementation in Modelica and giving several modeling and simulation examples.

2 Basic Physics and Mathematics of Quasi-Steady-State Fluid Flow

This section briefly describes conservation laws, constitutive relations and phenomenological empirical relations as they apply to *liquid* storage and flow in equipment as typically installed in process plants. Note, liquid density ρ is considered constant throughout the text.

2.1 Fundamental Relations for Liquid Storage and Flow

The *mass balance* for liquid storage is

$$\frac{dM}{dt} = \sum_i \dot{m}_i \tag{1}$$

(with total mass M contained within the reservoir and in- and outflow rates $\dot{m}$) and the relation describing *pressure drop* as a function of volumetric flow rate q is

$$\Delta p = f(q). \tag{2}$$

The well know Bernoulli equation in its original form relates *mechanical energies* of a fluid neglecting friction and considering the fluid as incompressible. It can be extended to include friction (*irreversible* loss of pressure head as energy dissipation) as well as addition of flow energy (e.g., by means of pumps or compressors). The sum of pressure-, velocity-, elevation-, friction- and pump-head remains constant along a flow trajectory (eq. 3, subscripts fr and pu for "friction" and "pump" respectively). According to the second law of thermodynamics, there is a restriction on the conversion direction of friction head, it cannot be converted back into other heads without interaction with the environment.

$$\frac{p}{\rho} + \frac{v^2}{2} + gz + \sum \Delta p_{fr} + \sum \Delta p_{pu} = const. \tag{3}$$

2.2 Fluid Reservoirs

For a container with constant cross section A, the *liquid level* obeys

$$\frac{dh}{dt} = \frac{1}{A} \sum_i q_i. \tag{4}$$

If liquid flows via a pipe and flange (velocity v_{pipe}) into a large[5] vessel (see fig. 1), the velocity head of the inflowing fluid can be considered irreversibly lost due to turbulent friction (see e.g., [Th99]), i.e., no pressure is recovered by slowing (process inside the vessel) the fluid to assumed flow velocity zero[6] in the vessel itself[7].

Figure 1: *Inflow to a vessel*

For *inflow* to a tank, extended Bernoulli can be formulated as

$$p_{vessel} = p_{pipe} + \frac{\rho}{2} v_{pipe}^2 - \Delta p_{fr,inlet}. \tag{5}$$

As indicated, the dynamic pressure is irreversibly lost with inflow, therefore, eq. 6 and 7 are valid.

$$\Delta p_{fr,inlet} = \frac{\rho}{2} v_{pipe}^2 \tag{6}$$

$$p_{vessel} = p_{pipe}. \tag{7}$$

Irreversible pressure loss involved with *outflow* of liquid at a flange of a vessel can be formulated as

$$\Delta p_{fr,outlet} = K_{con} \frac{\rho}{2} v_{pipe}^2, \tag{8}$$

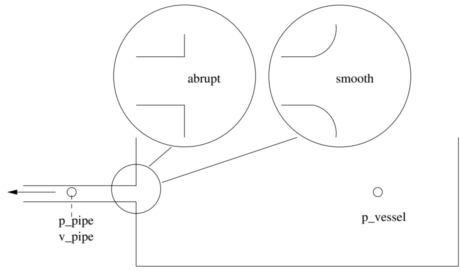

Figure 2: *Outflow from a vessel*

and is strongly dependent on the geometric form of the flange (see fig. 2). According to [Th99], the contraction coefficient K_{con} of an abrupt exit from the vessel to the outflow pipe is $K_{con,abrupt} \approx 0.5$ whereas for smooth, tapered outlets it is rather small $K_{con,smooth} \approx 0.05$.

[5] "Large" in the sense of the tank diameter being much larger than the flange diameter.

[6] Velocity "far" away from the inlet to the tank where the fluid is essentially not moving and undisturbed by turbulence from the inflow process.

[7] This is assumed true for both fluid inlets below and above the surface of the liquid contained in the vessel.

Pressure in the pipe and vessel relate for outflow as follows

$$p_{vessel} = p_{pipe} + \frac{\rho}{2} v_{pipe}^2 + \Delta p_{fr,outlet}, \tag{9}$$

which can alternatively be formulated with volumetric flow rate q to

$$p_{pipe} = p_{vessel} - \frac{\rho}{2A_{pipe}} (1 + K_{con}) q_{pipe}^2. \tag{10}$$

Note, the relations for pressures and flow velocities are different for the cases of in- and outflow (eq. 7 and 10). In reality, a physical flange at a vessel can normally carry both in- and outflows depending on the surrounding pressure situation. Therefore, in a tank model, a case distinction must be made in order to determine the pressure drop relation valid for the respective current flow situation. In this text, flow *into* a component is always taken positive ($q > 0.0[m^3/s]$), in accordance with Modelica conventions.

2.3 Flow Resistors

When a fluid flows through a flow conduit, frictional effects lead to pressure drops along the flow trajectory. In many flow armatures, e.g., pipe elbows and bends, orifices, diffusers and nozzles, the relation between pressure drop and flow velocity can be described by eq. 11 with pressure drop coefficient ζ as a function of Reynolds number Re and the geometry of the flow channel (eq. 12). In technical applications, ζ is often assumed constant for varying flow rate for many flow armatures.

$$dp = \zeta \cdot \frac{\rho}{2} \cdot v^2 \tag{11}$$

$$\zeta = \zeta(Re, geometry) \tag{12}$$

2.3.1 Pipes

The pressure drop in a pipe is customarily described by

$$\Delta p = \lambda \cdot \frac{L}{D} \cdot \frac{\rho}{2} v^2 \tag{13}$$

with pipe length L, pipe diameter D, flow velocity v and pipe friction factor λ. Depending on the magnitude of Re in the pipe

$$Re = \frac{|v|D}{\nu}, \tag{14}$$

different relations are to be used for λ, see table 1. The linear relation for laminar flow regime is

$$\lambda_{lam} = \frac{64}{Re}. \tag{15}$$

Re	**flow regime; relation**
$Re < 2300$	laminar; linear
$2000 < Re < 4000$	transient
$Re > 4000$	turbulent; e.g., Blasius, Colebrook Prandtl/Karman/Nikuradse

Table 1: *Flow regimes*

In the turbulent region and for smooth pipes[8], the Blasius relation can be used (eq. 16). Colebrook, Karman/Nikuradse and Prandtl/Nikuradse are all implicit relations, less handy to employ and are therefore not further discussed here.

$$\lambda_{turb} = 0.364 \cdot Re^{-\frac{1}{4}}. \tag{16}$$

2.3.2 Valves

A valve shall allow to control fluid flow by changing the valve opening and as a consequence the flow resistance across the valve. Usually the coefficients k_v and k_{vs} are used with valves; k_v indicates how much fluid–usually in $[m^3/h]$–passes the valve at an outer pressure gradient of $\Delta p = 1$ [bar] at a certain opening position of the valve and k_{vs} indicates the flow when the valve is fully open. The relation for the fully open valve is given in eq. 17.

$$q = k_{vs} \cdot \sqrt{|\Delta p|} \cdot sign(\Delta p) \tag{17}$$

A continuous control valve shall enable to control fluid flow over the whole continuous range of opening positions possible in the valve. k_v in this case is a function (eq. 18) of the valve opening position x (normalized to [0..1]) and k_{vs} and has a characteristic depending on the type and construction of the control valve (e.g., linear, equal-percentage).

$$k_v = k_v(k_{vs}, x) \tag{18}$$

Power control valves are driven by valve positioners (servo), which can be described by a first order exponential lag with time delay τ, relating actual valve travel x to demanded valve travel x_d by

$$\tau \frac{dx}{dt} = -x + x_d. \tag{19}$$

2.4 Pumps

Pumps can be seen as compensators for pressure drops to drive a fluid through its flow channel. Two idealized pump characteristics are shown in fig. 3 and 4. An *ideal flow source* is an abstraction of the behavior of volumetric pumps (piston, displacement pump), which have a very steep relation between pressure increase and flow across the pump. The idealized characteristic

[8]Most commercial pipes for process industry applications can normally be considered "smooth", if not, the Colebrook relation must be used which accounts for relative roughness ϵ/D.

is simply $q_{pump} = q_{source}$, independent of the pressure gradient. The other idealized representation is that of an *ideal pressure source* (centrifugal pump type). Its parameter can be set as height Δh_{source} (head rise), which determines the pressure rise in the pump (independent of the flow rate).

$$\Delta p_{pump} = \Delta h_{source} \cdot \rho \cdot g \tag{20}$$

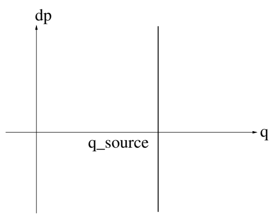

Figure 3: *Flow source*

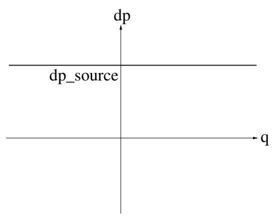

Figure 4: *Pressure source*

More detailed and realistic pump models are described in the literature and not explicitly discussed here due to lack of space. A model for a centrifugal pump is e.g., presented in [Ge85] as a first order model with nonlinear algebraic constraint equations.

3 Modelica Library Implementation

Having described the basic physics, this section is concerned with fluid flow component modeling to created a Modelica library. Its structure is organized in compliance with Modelica rules, grouping interfaces, various component types and example models in different packages, see fig. 5.

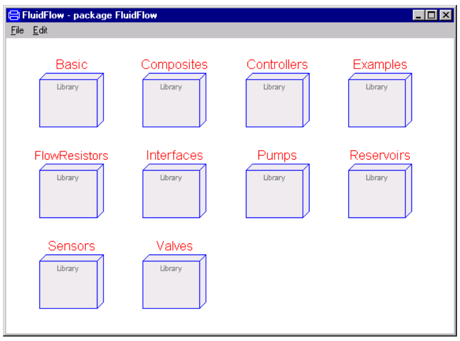

Figure 5: *Library structure*

3.1 Connector, Boundary Conditions and Fluid Properties

A connector called "Flange" (fig. 6) defines the potential variable p for pressure and the flow variable q for volumetric flow rate:

```
connector Flange
      SI.Pressure p;
  flow SI.VolumeFlowRate q;
end Flange
```

Currently, fluid properties are considered constant for all library components. The respective parameters are defined in an abstract class and given here, for the case of water:

```
partial model Fluid
  constant SI.Density rho=1000.0;
  constant SI.KinematicViscosity nu=1.0e-6;
end Fluid
```

Boundary conditions can either be set for pressure or for flow, the class icons are shown in fig. 7.

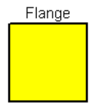

Figure 6: *Connector*

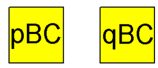

Figure 7: *Boundaries*

3.2 Flow Resistors

The components presented in this subsection are all modeled as purely resistive, i.e., no mass capacitance and–as indicated earlier–no momentum balance is formulated.

3.2.1 Pipes

With eq. 13 for pressure drop in a pipe and with eq. 15 for friction factor λ_{lam}, a linear relation for pressure drop Δp_{lam} in laminar pipe flow results as

$$\Delta p_{lam} = k_{lam} \cdot v \tag{21}$$

with coefficient

$$k_{lam} = 0.32 \cdot D^{-2} \cdot \nu L \rho. \tag{22}$$

For turbulent flow, the respective non-linear relation is

$$\Delta p_{turb} = k_{turb} \cdot sign(v) \cdot |v|^{7/4} \tag{23}$$

with

$$k_{turb} = 0.182 \cdot D^{-5/4} \cdot \nu^{1/4} L \rho. \tag{24}$$

The question of how to model the transient region (Re = [2300..4000]) arises. In reality, the flow will change from laminar to turbulent depending on the particular pipe geometry, flow disturbances, surface particularities in a somewhat random and discontinuous fashion. Here, a linear model is used to connect laminar to turbulent flow behavior, according to eq. 25 and 26 for positive and negative flow velocity respectively[9].

[9] Of course, other approaches are possible as well, in particular some with "smooth" transfers, but this linear model is feasible for the investigation purposes in mind.

$$\Delta p_{trans} = -k_{1trans} + k_{2trans} \cdot v \tag{25}$$

$$\Delta p_{trans} = k_{1trans} + k_{2trans} \cdot v \tag{26}$$

The two coefficients k_{1trans} and k_{2trans} can be calculated satisfying the conditions (eq. 27, 28) at the flow regime transition points. Depending on the current flow velocity, the flow regime is determined in the pipe model using the "if-statement" of Modelica for automatic detection of transition points (state events).

$$\Delta p_{lam}|_{Re=2300} = \Delta p_{trans}|_{Re=2300} \tag{27}$$

$$\Delta p_{trans}|_{Re=4000} = \Delta p_{turb}|_{Re=4000} \tag{28}$$

If the pipe connects flanges of different geographical elevations, an additional term Δp_g is included in the pipe model to account for gravitational pressure difference

$$\Delta p_g = \rho g \Delta z. \tag{29}$$

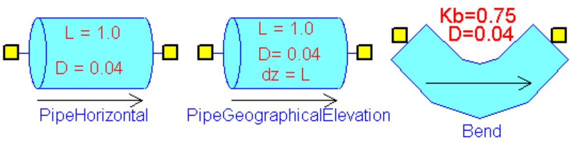

Figure 8: *Horizontal and elevated pipe; bend*

Fig. 8 displays the pipe component icons. The arrow is intended to indicate the default positive flow direction of the fluid in the pipe. This, in order to facilitate setting reasonable starting values for flow velocity to help the execution algorithms find consistent initial values at the beginning of a simulation.

3.2.2 Bends

The pressure drop across pipe bends (fig. 8, on the right) can be formulated as multiples of velocity heads (subscript "b" for bend)

$$\Delta p_{fr,b} = k_{bf} \frac{\rho}{2} v_b^2. \tag{30}$$

[Th99] lists some numerical values for k_b, see table 2.

type of bend	frictional loss k_b
Standard 45° bend	0.35
Standard 90° bend	0.75
180° bend	2.2

Table 2: *Examples of friction factors for pipe bends*

3.2.3 Valves

Valves for different valve characteristics are modeled. The one depicted in fig. 10 has a linear characteristic $k_v = k_{vs} \cdot x$ (fig. 9) with a first order servo for the valve positioner. Note, to avoid numerical problems, the valve is modeled to always have a small leakage[10], even for an input signal demanding for complete valve closure. The respective minimum opening valve travel x_{min} can be set to zero if desired and if feasible with the system model topology.

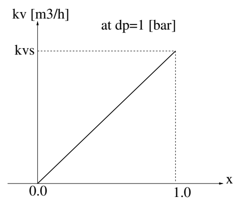

Figure 9: *Linear char.*

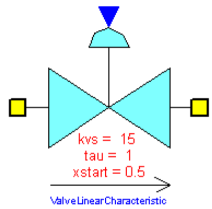

Figure 10: *Valve*

3.2.4 Other Flow Resistors

An idealized linear (eq. 31) and a general quadratic resistor (eq. 32) are implemented as well.

$$\Delta p_{lin} = k \cdot v \tag{31}$$

$$\Delta p_{gen} = \zeta \frac{\rho}{2} v_{bf}^2. \tag{32}$$

The linear resistor can be useful for simulation test purposes, e.g., when nonlinearities in a model cause problems calculating consistent initial conditions. The pressure loss coefficient ζ can be chosen in order to model orifices, venturi pipes or any other armature for which the pressure loss coefficient is known. Standard texts on fluid dynamics, e.g., [Yo01] or publications from flow armature manufacturers list loss factors for different forms of armatures.

3.3 Pumps

Fig. 11 shows icons of pumps modeled as ideal flow and pressure source as well as a more detailed centrifugal pump model.

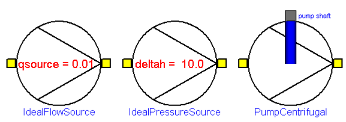

Figure 11: *Pump models*

[10] Possibility of small leakage is also implemented in other armatures allowing otherwise for complete flow interruption.

3.4 Tanks

A variety of tanks have been modeled. Here, a tank with constant cross section, open to atmosphere with a flange at the top and one at the bottom is illustrated. The pressure distribution in such a tank is given in eq. 33 (liquid level h, vertical elevation z in the liquid space, pressure p_s at the surface of the liquid).

$$p(z) = (p_s + \rho g h) - \frac{1}{\rho g h} \cdot z \qquad (33)$$

For an open tank, surface pressure equals ambient pressure $p_s = p_\infty$. The pressure at the bottom of the open tank therefore is

$$p|_{z=0} = p_\infty + \rho g h. \qquad (34)$$

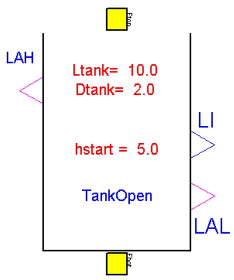

Figure 12: *Open tank*

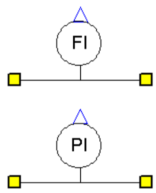

Figure 13: *Sensors*

Fig. 12 gives a graphical representation of this tank model. Output connectors are added to signal tank level (LI) as well as low and high level alarms (Boolean signals; LAL, LAH). Note, this tank model imposes no constraints on its level and does allow both liquid in- and outflow at its lower flange, depending on the gradient of inner to outer pressure conditions. Clearly, the upper flange is always above the liquid surface in the tank (unless the tank is completely full), and therefore, no liquid outflow is possible at the top.

3.5 Additional Models

A variety of additional component models were created, among them, sensors (fig. 13 shows flow and pressure indicators, realized with or without sensor dynamics), no-return valves (analog to the diode in the electric domain), various switches and commutators to control fluid routing, pipe diameter changes, tanks with constraints on levels and flow directions at it's flanges, pressurized tanks and relief valves. Some of the models are thoroughly tested, others have a somewhat experimental character.

4 Modeling and Simulation Examples

A few–rather simple–models shall first be given to demonstrate the basic functionality of the library, before progressing to more comprehensive applications.

4.1 Introductory Demonstration Models

Tank Emptying Fig. 14 shows a model consisting of a tank with a pipe connected to its lower flange. Boundary conditions set the pressure at the outlet of the pipe to ambient pressure and the inflow rate at the upper flange to zero. Initial tank level is $h_s = 5.0m$. As expected, during simulation, the tank level decreases and it can be seen in fig. 15 that the tank becomes empty after about $6000s$ (pipe of $4cm$ inner diameter and $10m$ length).

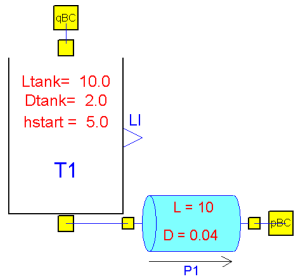

Figure 14: *Model one*

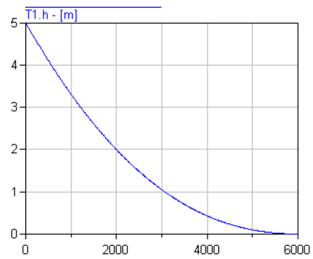

Figure 15: *Emptying*

Tank Level Equalization In the next model, two tanks of the same dimensions are connected with a pipe at their lower flanges (fig. 16). Initial levels are $h_{1,s} = 8.0m$ and $h_{2,s} = 2.0m$. There is no inflow to the tanks at their upper flanges. During simulation, the levels approach and equalize, as can be seen in fig. 17.

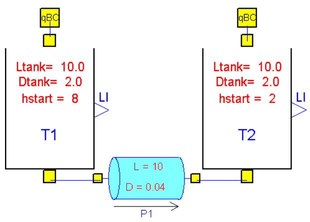

Figure 16: *Model two*

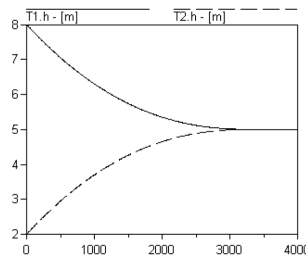

Figure 17: *Equalization*

Flow Inversion in a Pipe The model of fig. 16 is used again. This time, rather strong liquid inflow at the upper flange of tank 2 is imposed as a step $q_{2,in} = 0.01m^3/s$ at time $t = 1000s$. Fig. 18 and 19 show the tank levels, the inflow step and the flow rate in the connecting pipe. As can be seen, the behavior of the model is initially identical to the one illustrated above, after $1000s$, the level in tank 2 increases faster due to the liquid added at its upper flange and surpasses the level of tank 1 after about $1550s$, at which point in time the flow in the pipe is inverted. The simulation runs without numerical trouble through the point of flow inversion.

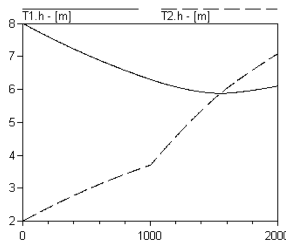

Figure 18: *Tank levels*

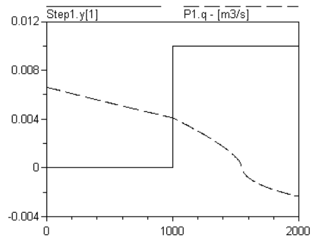

Figure 19: *Step, flow*

4.2 Laboratory Test-bed

A somewhat larger and more complex model is made of a laboratory test-bed which is currently installed at our institute. It consists of three tanks, a variety of connecting horizontal and vertical pipe segments, a pump and four continuous control valves. Fig. 20 depicts the PI[11] flow diagram, fig. 21 gives a 3-D view (CAD-draw from the planning phase) and fig. 22 shows the test-bed in its recent early commissioning phase[12]. A respective Modelica/Dymola model is shown in fig. 23.

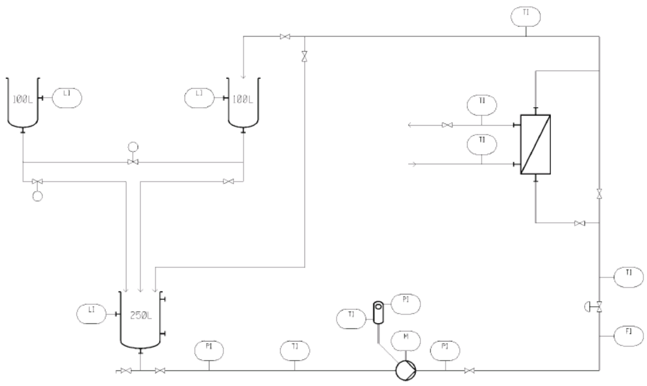

Figure 20: *PI scheme of test-bed*

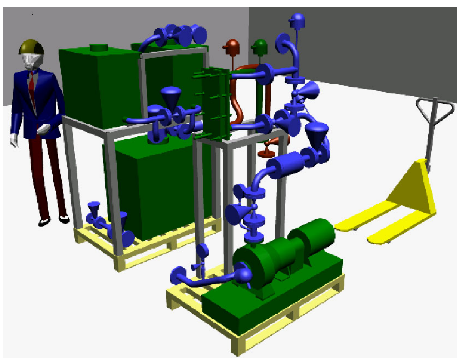

Figure 21: *3-D picture of the test-bed*

For control scheme investigation, one flow ("FC" for flow control) and two level ("LC") controllers are included in the model (PID-type controllers with limited output and anti-windup from the standard Modelica library with continuous control valves as actuators). The valves all have positioning dynamics (1st-order lag) with time constants $\tau = 1s$ (fast valve with pneumatic drive) and $k_{vs} = 40m^3/s$ for LC and $k_{vs} = 15m^3/s$ for FC. LC shall keep the levels in the upper tanks "Tleft" and "Tright" at their desired set-points ($T_{left,sp} = 0.4m$, $T_{right,sp} = 0.5m$). FC is used to control the flow rate through the pump (centrifugal pump, modeled as an ideal pressure source with hydraulic head of $\Delta h_{pump} = 80m$). After some simulation experiments, PID control parameters (gain k, integrative and derivative time constants T_i and T_d) were chosen as indicated in table 3.

[11] Process and Instrumentation.

[12] The design in the flow diagram and the actual realization of the test-bed differ somewhat, but this is not of importance here.

Figure 22: *Test bed: Commissioning phase*

LC	k	50
	T_i	5
	T_d	0.1
FC	k	100
	T_i	5
	T_d	0.1

Table 3: *Controller parameters*

Fig. 24 and fig. 25 show the upper tank levels and the respective control valve positions for a simulation experiment of 400s duration. Initial levels of the upper tanks are set to $h_{left,s} = 0.3m$ and $h_{right,s} = 0.6m$. A step is imposed on the set-point of the flow controller, at time $t = 200s$ (increase from $q_{sp1} = 0.00175$ to $q_{sp2} = 0.00275m^3/s$). With the controller parameters given above, the levels are kept at their set-points in a satisfactory fashion.
It can be seen in fig. 23, the system topology (as illustrated in the PI flow diagram and on the fotograph) is maintained in the Modelica model. The model presents itself in a graphical manner so that its structure can be very quickly and intuitively understood. This is inherent to the physical object-oriented modeling paradigm

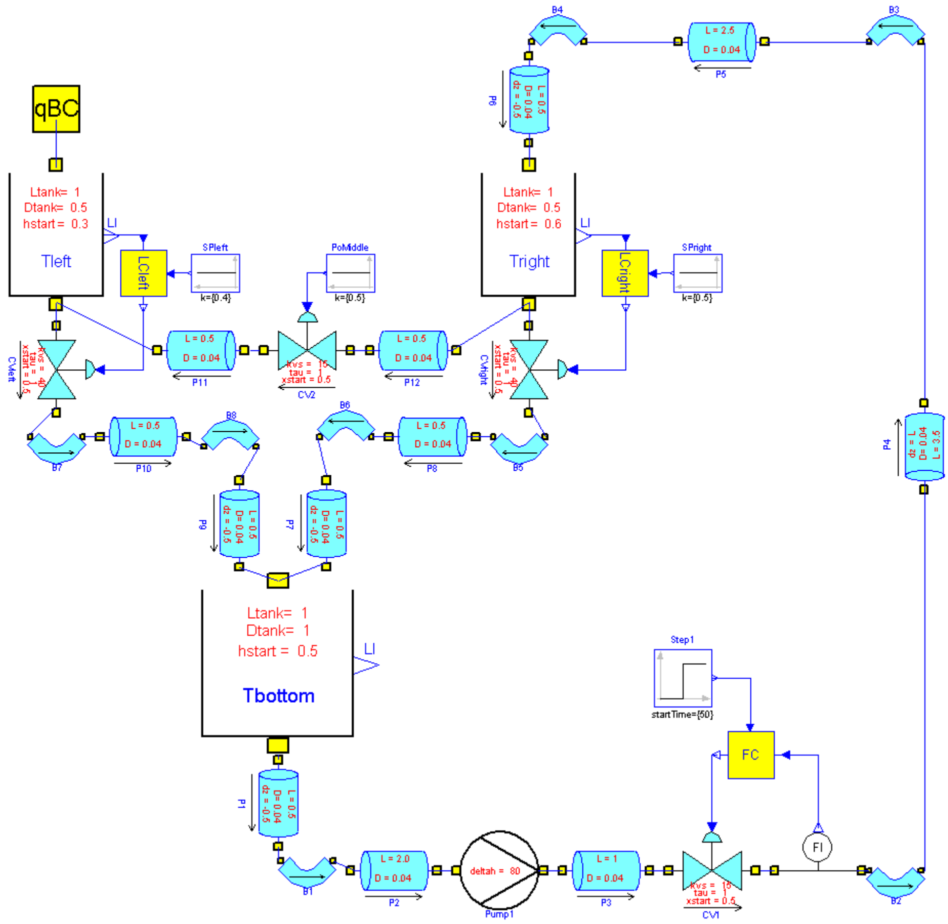

Figure 23: *Dymola model of testbed*

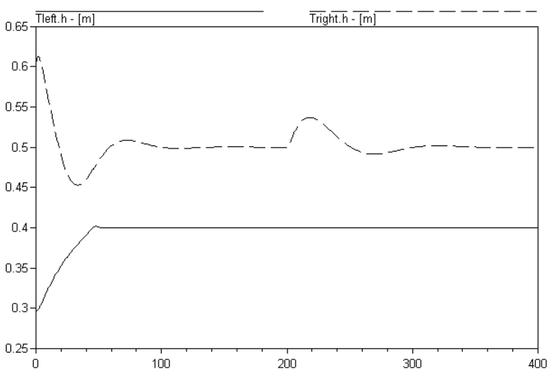

Figure 24: *Levels in the upper tanks*

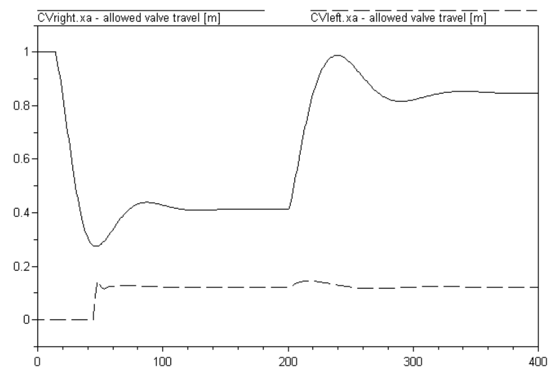

Figure 25: *Level control valve positions*

of Modelica and regarded as very beneficial. The effort necessary to compose the test-bed model with the library presented was minor. Compare this to the workload if the modeler had to analytically and manually derive the overall system equations! Such a proceeding would probably be time-consuming and error prone even for this still rather simple three-tank model, especially because there is non-linearities and hybrid phenomena to account for as well. The library therefore can greatly reduce the modeling burden and increase efficiency of carrying out engineering design tasks (in this case, controller design and investigation of dynamic behavior).

Furthermore, it has been shown (e.g., in [Ti00]) that the Modelica modeling approach allows to scale models to many thousands, if not hundreds of thousands of defining equations. This is of great importance if trying to model large and complex systems.

The presented test-bed is not yet operational in reality; it will be interesting to validate the model against experimental data and possibly refine it at a later time.

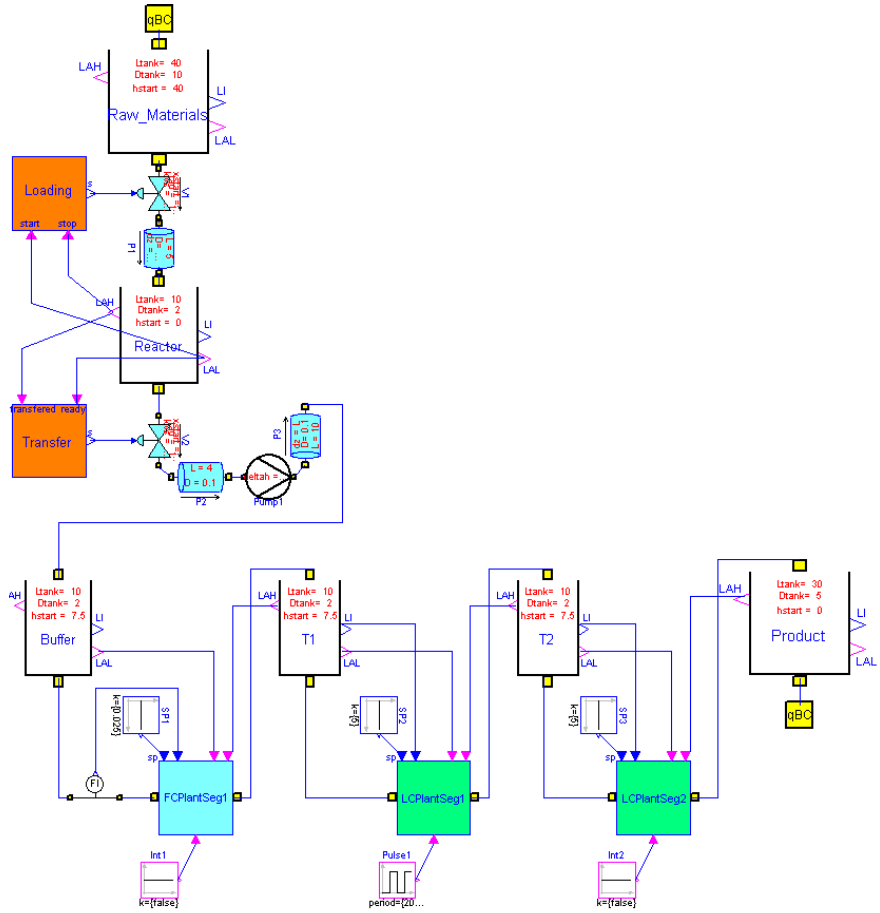

Figure 26: *Plant model top view*

4.3 Modeling of Mass Flow in a Process Plant

For purposes of maintenance management in process plants, it is advantageous to have a good knowledge of plant dynamics. Process plants often can be considered as interconnected flow segments where the linking elements are vessels[13]. Since the flow segments are decoupled from each other to some degree (depending on the sizes of intermediate buffer vessels as well as on the throughput capacities of flow segments), it can be beneficial to take mass flow dynamics into account when defining maintenance strategies and scheduling maintenance tasks.

Fig. 26 illustrates a model of a plant with both a batch and continuous part, consisting of a tank with raw materials, a reactor, a buffer tank enabling synchronization between batch and continuous part, two intermediate tanks in the continuous part and a large storage vessel for the final product. Note, it is not necessary to see all the details in fig. 26, rather, the aim is to illustrate the overall plant structure and the modeling concept.

The loading of the reactor with raw material is organized by control logic in the block "Loading" and the transfer of the reactor content after reaction is completed is controlled by block "Transfer"; the internals of the latter are shown fig. 27. As can be seen, the control logic is realized with Petri net formalism, based on the Modelica library described in [Mo98]. In particular, the reaction duration is modeled as delayed transition firing (transition "TReactionDelay")[14].

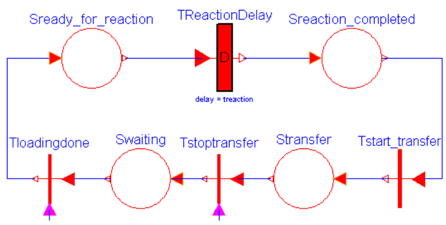

Figure 27: *Transfer control logic*

Two types of flow segments are defined, namely, a flow and a level controlled variant ("FCPlantSeg", "LCPlantSeg"). Without going into details, it shall be said

[13] An abstraction into flow and storage elements as basic modeling blocks is extensively used in systems dynamics, e.g., see [Fo61].

[14] The Modelica Petri net library was extended in this context, supporting timed stochastic Petri nets and places with multiple token capacity, this aspect will be published in the near future.

here, the segments can contain whatever non-storage library component presented so far, but normally consist of at least a flow driver (pump), flow resistor (process steps and pipes) as well as control logic. The flow segment blocks receive measured flow or level signals, reference values as well as level alarms from neighboring vessels as inputs. In addition, an external Boolean signal can be supplied to indicate flow interruption, which can be useful to include deterministic or stochastic component and subsystem failure models in the plant model.

A simulation experiment with a flow interruption in the middle flow segment ("LCPlantSeg1") is carried out for a total simulation duration of 3000 time units. Fig. 28 shows the resulting tank levels, it can be seen how the level in the reactor and the subsequent buffer tank fluctuate. As well, the effect and propagation of the flow interruption (1000 to 1800 time units) in the plant is shown.

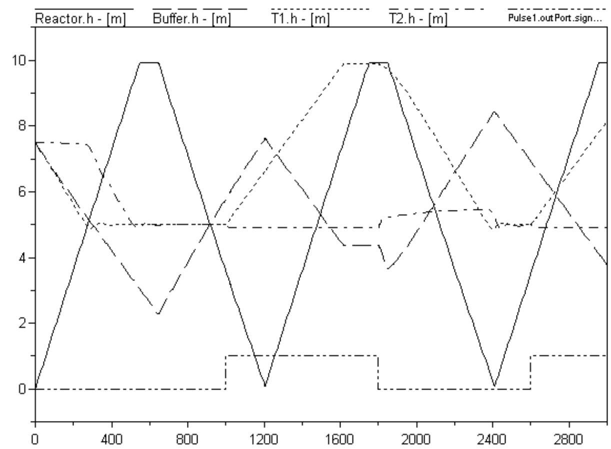

Figure 28: *Tank levels in the plant*

Plant control strategy, flow segment throughput capacities and tank sizes all influence the sensitivity of the plant to interruptions (e.g., caused by component failures or maintenance action) in flow segments , which can be analyzed with models as just described. The situation of course is yet more interesting if internal feedback loops are present in the plant.

5 Conclusion and Outlook

A library for mass flow simulation in process plants was presented and it has been shown how it can be used to efficiently generate models of possibly large and complex systems.

The presented plant models could be extended to include important energy exchanging equipment (heaters, coolers), more detailed component models as well as stochastic Petri nets for component failure and repair processes.

An important question to be dealt with in the future, is how to efficiently handle the great bandwidth of characteristic times in a system such as a process plant. E.g., components often have life-times (between component failures or preventive overhauls) in the range of month to years, whereas the time constants of buffer tanks are minutes to hours, the controller and actuator dynamics seconds to minutes. If models were to be used for maintenance strategy optimization accounting for plant mass flow dynamics, it is desirable to have models which allow for rapid progress in simulation time for normal, nominal system behavior, switching to others, more detailed ones, in the case of faults or failures; multi-mode models are needed for this.

Another non-trivial topic is initial value calculation, especially as here for the case of quasi-steady state flow models, where nonlinear algebraic equations must be solved for iteratively, to calculate consistent initial conditions. The tool Dymola seems to be quite sensitive to choice of starting values, which is inconvenient in large models. It is hoped, the tool will be further equipped with even stronger algorithms in the future to support the simulation analyst in this respect.

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