CHEMICAL ENGINEERING TRANSACTIONS

VOL. 32, 2013

A publication of AIDIC
The Italian Association of Chemical Engineering
Online at: www.aidic.it/cet

Chief Editors: Sauro Pierucci, Jiří J. Klemeš

ISBN 978-88-95608-23-5; **ISSN** 1974-9791

DOI: 10.3303/CET1332212

Systematic Modelling of Flow and Pressure Distribution

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In any plant, it is the pressure that drives convective flow of mass from one part to another. A systematic method of modelling the flow and the pressure distribution is derived based on a finite-volume approached captured in a graph. This approach is conform with our network modelling method "visual modelling".

1. Background

Most process models are based on a network of finite volumes. Chemical engineers refer to it as the control-volume approach (Preisig, 2010). We look at the network as a graph, where the volumes represent the capacities and the arcs the transfer of extensive quantities, more precisely mass flow, usually a vector of component mass flows, energy flow, usually conductive and radiation heat flow, mechanical work, volume work and the like. Whilst mass has a considerable inertia, the pressure distribution is happening at the speed of sound, thus comparatively very fast. In most cases, the dynamics of the pressure distribution is not of interest in chemical processes and one assumes it to "just happen", technically speaking one assumes event-dynamics. The exception is the description of explosions, detonations – any system that operates on the time scale of pressure wave propagation in a system. But why do we need the pressure distribution? First reason is that convective flow is driven by the pressure difference and the second one is that the material properties are a function of pressure as it enters the equation of state and thus the energy functions.

2. A Sample System

To illustrate the approach, we introduce a simple, but representative common part of a plant (Fig. 1). It is a near barometric pressure inside. In addition the tank has a feed pipe connected to the water supply on the top, and the bottom outlet is connected to the drain at barometric pressure.
The mechanics of the process are apparent: As one puts water into the tank it starts filling up, whilst the water outflow is driven by the pressure in the tank. Latter is essentially the barometric pressure plus the hydrostatic pressure exerted by the water. The flow into the tank is a free jet that extends from the end of the pipe to the water surface. The purpose of the breathing pipe is to allow for air to go in and out of the tank so as to equalize the inside pressure with the outside pressure. This is a dynamic process and if the tank level changes fast, the breathing pipe's resistant will have the effect that the pressure inside and outside are not equal.

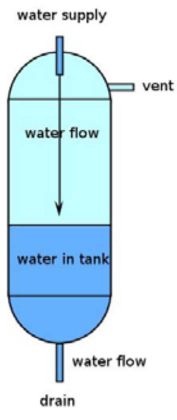

Figure 1: Sample process

The modelling of the process is done step by step with the first one being an abstraction of the plant as a network of capacities and flows of extensive quantities.

2.1 A first topology

The modelling approach we call "visual modelling". The plant model is represented as a graph choosing the nodes to represent capacities and the arcs to represent flows of extensive quantities. When establishing this graph, we make the first set of time-scale assumptions.
Any system we describe uses three time domains, one in which the associated capacities are considered constant, one in which they are dynamic and change

Please cite this article as: Preisig H.A., 2013, Systematic modelling of flow and pressure distribution, Chemical Engineering Transactions, 32, 1267-1272 DOI: 10.3303/CET1332212

visibly with time, and one in which things just happen, being event-dynamic. The constant systems, we call reservoirs. Shown as half circles they are open on one side extending to infinity. For dynamic systems we have two cases to consider, namely distributed systems and lumped systems. Lumped systems are characterised by intensive properties not to be a function of the position in contrast to the distributed systems where the intensive properties are a function of the position. Both type of systems are of finite dynamic nature and are mathematically formulated as differential equations. Lumped systems are ordinary and distributed systems are represented by partial differential equations. In the third domain we have event-dynamic systems, which, when lumped are shown as simple bars and when distributed as rectangles. The initial topology always contains maximal information. Any change towards more detail requires an extension of the graph splitting capacities and adding more transfers, make the granularity of the model finer (Preisig, 2010). Our first and "maximal" graph is shown in Fig. 2. Here the oval nodes represent the distributed capacities as labelled, whilst the bars represent the boundaries between the respective capacities.

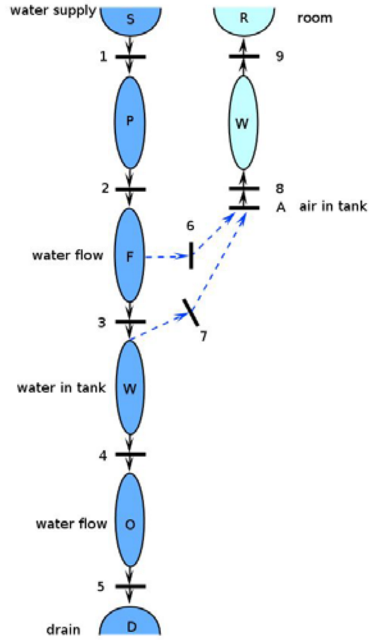

Figure 2: A first graph

2.2 More time-scale assumption

Further simplifications are based on additional time-scale assumptions. In this case, the next step requires a split of the plant model into two separate time scales. Since we assume that the pressure wave propagate very fast, we get an event-dynamic model for the pressure distribution, whilst the dynamics of the mass distribution happens in the "visible" dynamic range. Both are embedded in a set of reservoirs that represent the process-embedding environment, which are considered constant in terms of their intensive properties and infinitely large in terms of their capacity. So we first split the description into a model for the event-dynamic part and the dynamic part, the first one being the momentum propagation and the second the mass.

The left part of Fig. 3 shows the event-dynamic model, the right the dynamic model. As mentioned, we use rectangles for the distributed capacities and circles for the lumped system. The black rectangles show systems that reduce to a plug-flow only and are reduced to a simple dead-time for the transport; whilst the coloured rectangles also consider the distribution in the intensities, in particular the pressure. The time-scale assumptions can be extended as demonstrated on the water jet, where on the right-hand-side it is assumed instantaneous so no significant dead-time associated with the water passing from the end of the pipe to the surface, whilst on the left-hand-side, it is modelled as an event-dynamic distributed system. We could consider making the same assumption for the pipes, thus the water pipe in and out and the breathing pipe. This then results in what most people would probably write as their very first model for the behaviour of the plant in terms of mass, namely, water accumulated per unit time in the tank is the difference between what is coming in and what is going out.

3. Model Equations

The mathematical model is assembled from the models of the capacities and the model of the transfers. The equations for the different parts are collected in the table below. The table's first column contains a description of the model component, the second introduces a label for each equation which we use below to discuss the overall equation pattern. The third contains the equation.

The first equation describes the mass conservation in vector form for a single homogeneous material for a lumped system. It simply says that the accumulation is equivalent to the sum of all the physical inflows minus the physical outflows. The representation makes use of the underlying directed graph for the physical topology. There we introduce the reference co-ordinates for each flow, represented by the directed arcs, the arrows. The matrix $\underline{\mathbf{F}}_s$ is the row of the incidence matrix of the graph for system *s*. The incidence matrix has as row the nodes (systems / capacities) and in the columns the arcs (transports). So for the mass balance of the tank the mass conservation equation $\mathbb{M}_T$ is $\dot{m}_T = \hat{m}_{3|W} - \hat{m}_{W|4}$.

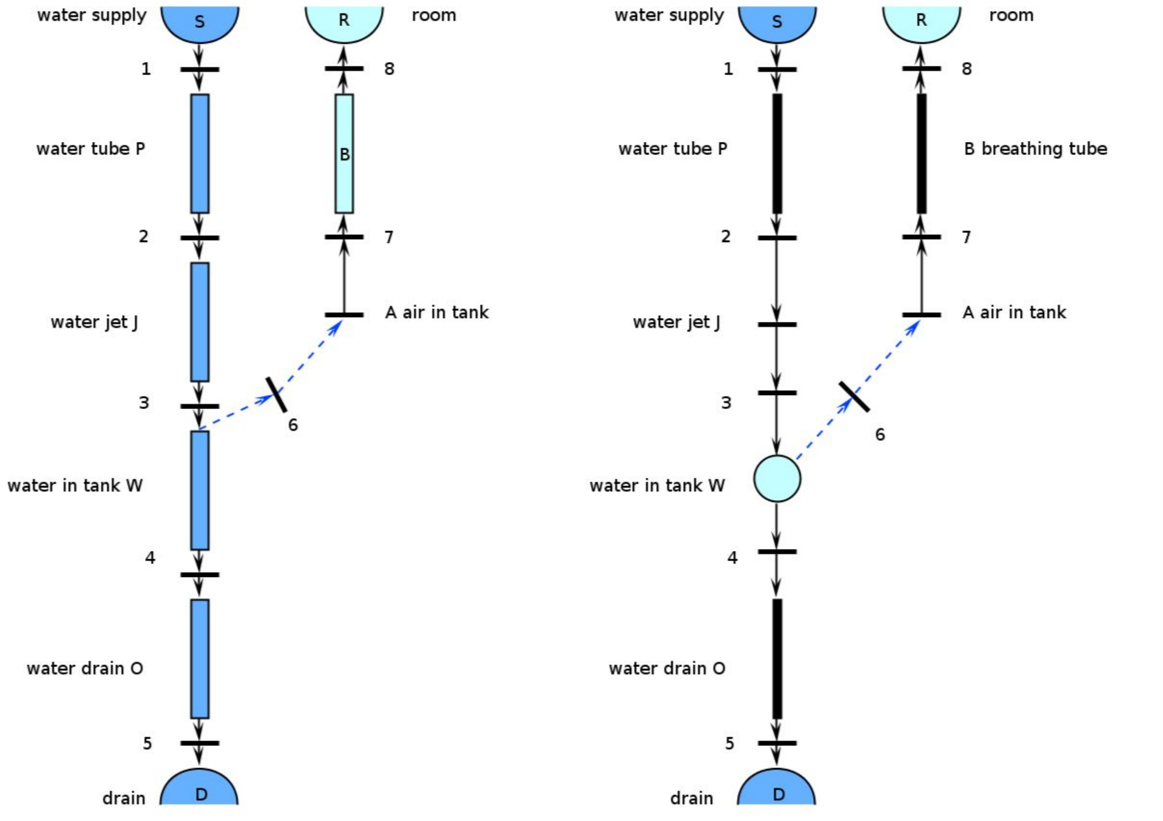

Figure 3: Splitting the time-scales: left event-dynamic, right dynamic

Note on how we use the indexing scheme to indicate the flows and its direction: The source is the first part of the index using the identifier of the system being at the tail of the directed arc. The vertical bar is the separator and the second index is the identifier of the sink, the head of the directed arc. The row for the fluid in the tank of the incidence matrix thus is all zeros except the columns for the flow *3|W* and *W|4*.
For the pressure distribution we use the event-dynamic model for which the slow model is entering as a snap shot, that is, an implicit singular perturbation is done assuming a "pseudo steady state" for the tank's mass. The geometry relates the volume to the level in the tank and the material properties related the state mass to the volume, which is one of the critical pieces of information required.

Table 1Model equations

Component description	**Symbol**	**Equation**
Mass of lumped system	$\mathbb{M}_s^d$	$m_s := \int_0^t \dot{m}_s(\tau)\,d\tau + m_s(0)$
Mass balance lumped (dynamic capacity *s*)	$\dot{\mathbb{M}}_s^d$	$\dot{m}_s = \underline{\underline{\mathbf{F}}}_s\,\underline{\hat{\mathbf{m}}}$
Mass balance lumped / distributed event-dynamic	$\mathbb{M}_s^e$	$0 = \underline{\underline{\mathbf{F}}}_s\,\underline{\hat{\mathbf{m}}}$
Energy balance (dynamic capacity *s*)	$\mathbb{E}_s^d$	$\dot{E}_s = \underline{\underline{\mathbf{F}}}_s\,\underline{\hat{\mathbf{U}}} + \underline{\underline{\mathbf{F}}}_s\,\underline{\hat{\mathbf{K}}} + \underline{\underline{\mathbf{F}}}_s\,\underline{\hat{\mathbf{P}}} + \underline{\underline{\mathbf{F}}}_s\,\underline{\hat{\mathbf{w}}}^v - \hat{w}_s^f$
Energy balance (event-dynamic *s*)	$\mathbb{E}_s^e$	$0 = \underline{\underline{\mathbf{F}}}_s\,\underline{\hat{\mathbf{U}}} + \underline{\underline{\mathbf{F}}}_s\,\underline{\hat{\mathbf{K}}} + \underline{\underline{\mathbf{F}}}_s\,\underline{\hat{\mathbf{P}}} + \underline{\underline{\mathbf{F}}}_s\,\underline{\hat{\mathbf{w}}}^v - \hat{w}_s^f$
Mass flow	$\hat{\mathbb{M}}_m$	$\hat{m}_m :=_m \hat{V}_m$
Kinetic energy flow *m*	$\hat{\mathbb{K}}_m$	$\hat{K}_m := \hat{m}_m \frac{v_m^2}{2}$
Potential energy flow *m*	$\hat{\mathbb{P}}_m$	$\hat{P}_m := \hat{m}_m\,g\,h_m$

Component description	**Symbol**	**Equation**
Volume work flow *m*	$\hat{\mathbb{W}}^v_m$	$\hat{w}^v_m := p_m\, \hat{V}_m$
Friction work over transport system *s*	$\hat{\mathbb{W}}^f_m$	$\hat{w}^f_m := \underline{\underline{\mathbf{F}}}_M\, p^f_m\, \hat{V}_m$
Pressure drop due to friction transport system *s* for cylindrical geometry and incompressible fluid Darcy-Weisbach model	$\hat{\mathbb{F}}_m$	$\Delta p^f := \underline{\underline{\mathbf{F}}}_m p^f_m := f_m\, \frac{l_m}{d_m}\, \frac{v_m^2}{2}$
Friction factor model for laminar flow	$\mathbb{F}^l_m$	$f^l_m := f^l_m(Re_m) := \frac{64}{Re_m}$
Friction factor model for turbulent flow	$\mathbb{F}^t_m$	$f^t_m := f^t_m(Re_m, \epsilon)$
Friction factor model for highly turbulent flow	$\mathbb{F}^h_m$	$f^h_m := f^h_m(\epsilon)$
Reynold number	$\mathbb{R}e_m$	$Re_m := \left(\frac{\rho\, v_m\, d_m}{\mu}\right)$
Geometrical relation	$\mathbb{G}^v_m$	$v_m := A_m^{-1}\, \hat{V}_m$
Geometrical relation	$\mathbb{G}^A_m$	$A_m := \pi\, r_m^2$
Geometrical relation	$\mathbb{G}^d_m$	$d_m := 2\, r_m$
Geometrical relation	$\mathbb{G}^h_m$	$h_s := A_s^{-1}\, V_s$
Geometrical relation	$\mathbb{G}^V_s$	$V_s := h_s\, A_s$
Property	$\mathbb{P}_m$	$V_s := \rho^{-1}\, m_s$
Rigid container	$\mathbb{V}_s$	$0 = V^l + V^g$
Note that we distinguish between accumulation and flow. For the first we use the dot-decorator, whilst for the second the hat-decorator. Obviously both have the same physical units.		$\dot{x}$ :: accumlation of x $\hat{x}$ :: flow of x

The plant model consists of the components:

- The fluid being incompressible – for all practical purposes.
- Pipes that are assumed to be cylindrical.

Equations	$\mathbb{M}^e_s \quad \mathbb{E}^e_s \quad \hat{\mathbb{P}}_m \quad \hat{\mathbb{W}}^v_m \quad \hat{\mathbb{M}}_m$
Assumptions (A) Facts (F)	$\underline{\underline{\mathbf{F}}}_s\, \underline{\hat{\mathbf{U}}} \overset{A}{:=} 0$ cylindrical: $\underline{\underline{\mathbf{F}}}_s\, \underline{\hat{\mathbf{K}}} \overset{F}{:=} 0$
	$0 = \underline{\underline{\mathbf{F}}}_s\, \underline{\hat{\mathbf{P}}} + \underline{\underline{\mathbf{F}}}_s\, \underline{\hat{\mathbf{w}}}^v - \hat{w}^f_s \quad = \hat{m}_s\, g\, \underline{\underline{\mathbf{F}}}_s\, \underline{\mathbf{h}} + \rho^{-1}\, \hat{m}_s \underline{\underline{\mathbf{F}}}_s\, \underline{\mathbf{p}} - \mathbb{W}^f_s\left(\hat{m}_s\right)$ $= g\, \underline{\underline{\mathbf{F}}}_s\, \underline{\mathbf{h}} + \rho^{-1}\, \underline{\underline{\mathbf{F}}}_s\, \underline{\mathbf{p}} - \mathbb{W}^f_s\left(\hat{m}_s\right)/\hat{m}_s$

- Tank

Equations	$\mathbb{V}_s$
Constant volume	$0 = V^l_W + V^l_J + V^g_G$

- Tank event-dynamic liquid phase or gas phase:

Equations	$\mathbb{M}^e_s \quad \mathbb{E}^e_s \quad \hat{\mathbb{P}}_m \quad \hat{\mathbb{W}}^v_m \quad \hat{\mathbb{W}}^f_m \quad \mathbb{F}^{l\vert t\vert h}_m \quad \mathbb{G}^v_m\, \mathbb{R}e_m$
Assumptions (A) Facts (F)	$\underline{\underline{\mathbf{F}}}_s\, \underline{\hat{\mathbf{U}}} \overset{A}{:=} 0$ cylindrical: $\underline{\underline{\mathbf{F}}}_s\, \underline{\hat{\mathbf{K}}} \overset{F}{:=} 0$ no friction: $\hat{w}^f_s \overset{A}{:=} 0$
	$0 = \underline{\underline{\mathbf{F}}}_s\, \underline{\hat{\mathbf{P}}} + \underline{\underline{\mathbf{F}}}_s\, \underline{\hat{\mathbf{w}}}^v \quad = \underline{\underline{\mathbf{F}}}_s\left(g\, \underline{\mathbf{h}} + \underline{\mathbf{p}}\right)$

- Ditto, but dynamic liquid phase:

Equations	$\mathbb{M}_s^d \quad \hat{\mathbb{P}}_m \quad \hat{\mathbb{W}}_m^v \quad \mathbb{G}_m^h$
Assumptions (A) Facts (F)	$\underline{\underline{\mathbf{F}}}_s \, \underline{\hat{\mathbf{U}}} :\overset{A}{=} 0$ cylindrical: $\underline{\underline{\mathbf{F}}}_s \, \underline{\hat{\mathbf{K}}} :\overset{F}{=} 0$ no friction: $\hat{w}_s^f :\overset{A}{=} 0$
	$0 = \underline{\underline{\mathbf{F}}}_s \, \underline{\hat{\mathbf{P}}} + \underline{\underline{\mathbf{F}}}_s \, \underline{\hat{\mathbf{w}}}^v = \underline{\underline{\mathbf{F}}}_s \, (g \, \underline{\mathbf{h}} + \underline{\mathbf{p}})$

- Ditto, but dynamic gas phase:

Equations	$\mathbb{M}_s^d \quad \hat{\mathbb{P}}_m \quad \hat{\mathbb{W}}_m^v \quad \mathbb{G}_m^h$
Assumptions (A) Facts (F)	Negligible: $\underline{\underline{\mathbf{F}}}_s \, \underline{\hat{\mathbf{U}}} :\overset{A}{=} 0$ cylindrical: $\underline{\underline{\mathbf{F}}}_s \, \underline{\hat{\mathbf{K}}} :\overset{F}{=} 0$ no friction: $\hat{w}_s^f :\overset{A}{=} 0$ negligible: $\underline{\underline{\mathbf{F}}}_s \, \underline{\hat{\mathbf{P}}} :\overset{A}{=} 0$
	$0 = \underline{\underline{\mathbf{F}}}_s \, \underline{\hat{\mathbf{w}}}^v = \underline{\underline{\mathbf{F}}}_s \, \underline{\mathbf{p}}$

- Free jet that is assumed to be cylindrical

Equations	$\mathbb{M}_s^d \quad \hat{\mathbb{P}}_m \quad \hat{\mathbb{W}}_m^v \quad \mathbb{G}_s^V$
Assumptions (A) Facts (F)	Negligible: $\underline{\underline{\mathbf{F}}}_s \, \underline{\hat{\mathbf{U}}} :\overset{A}{=} 0$ cylindrical: $\underline{\underline{\mathbf{F}}}_s \, \underline{\hat{\mathbf{K}}} :\overset{F}{=} 0$ no friction: $\hat{w}_s^f :\overset{A}{=} 0$ negligible: $\underline{\underline{\mathbf{F}}}_s \, \underline{\hat{\mathbf{P}}} :\overset{A}{=} 0$
	$0 = \underline{\underline{\mathbf{F}}}_s \, \underline{\hat{\mathbf{w}}}^v = \underline{\underline{\mathbf{F}}}_s \, \underline{\mathbf{p}}$

3.1 Assembling the model for the plant

In view of the page limits we continue with an event smaller, simplified version of the given plant: It consists of a series of flow units that transport an incompressible fluid. The model assembles from the mass and energy balance for the tubes and the boundaries between the tubes:

Pipes A,B,C	$\mathbb{E}_s^e \quad \mathbb{M}_s^e$	$0 = g \, \underline{\underline{\mathbf{F}}}_s \, \underline{\mathbf{h}} + \rho^{-1} \, \underline{\underline{\mathbf{F}}}_s \, \underline{\mathbf{p}} - \mathbb{W}_s^f \, (\hat{m}_s) \, / \hat{m}_s$
Interfaces 2,3	$\mathbb{M}_s^e$	$0 = \underline{\underline{\mathbf{F}}}_s \, \underline{\hat{\mathbf{m}}}$
Interfaces 2,3	$\mathbb{E}_s^e$	$0 = \underline{\underline{\mathbf{F}}}_s \, \underline{\hat{\mathbf{w}}}^v = \hat{V} \, \underline{\underline{\mathbf{F}}}_s \, \underline{\mathbf{p}} = \underline{\underline{\mathbf{F}}}_s \, \underline{\mathbf{p}}$

The plant's position in the state space is defined by the conditions on the boundaries, which in this case are the pressures at the interfaces 1 and 4. These are the pressures of the respective connected reservoirs. In more complex models, also the other intensive properties of the reservoirs enter the definition space, for example the composition. Further, we require the geometry of the pipe system, here we assumed cylindrical pipes. In addition we need the location of the interfaces in the space, thus the relative height measurements.
The mass balances for the interfaces equal the flows, thus there is only one overall flow in the system. The energy balances of the interfaces equal the pressure on either side of the interfaces. This leaves 3 quantities to be computed, namely the mass flow through the system and the pressures at the interfaces 2 and 3. These can be obtained from the three energy balances for the pipes.
For laminar flow systems, the friction term is linear in the mass flow. So one can rewrite the equations in a matrix format:

$$0 = g \, \underline{\underline{\mathbf{F}}} \, \underline{\mathbf{h}} + \rho^{-1} \, \underline{\underline{\mathbf{F}}} \, \underline{\mathbf{p}} - \hat{m} \, \underline{\mathbf{c}}^f$$

with the vector $\mathbf{c}^f$ being a vector of constant friction coefficients.

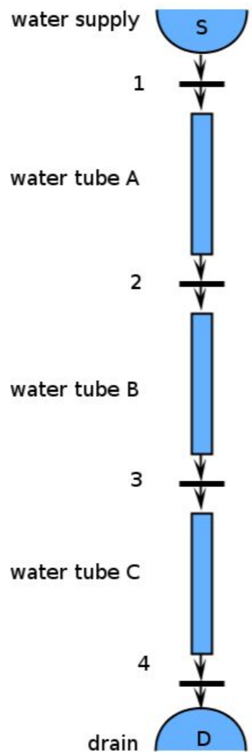

Figure 4: Pipes only

The open tank adds the element of branching in the network and one of the nodes being dynamic with respect to mass, namely the contents.

Capacities	$\mathbb{E}_s^e$ $s := P,\ J,\ W,\ O,\ A,\ B$ $\mathbb{M}_s^e \& \mathbb{P}_s$ $s := P,\ J,\ O,\ B$	$0 = g \, \underline{\underline{\mathbf{F}}}_s \, \underline{\mathbf{h}} + \rho^{-1} \, \underline{\underline{\mathbf{F}}}_s \, \underline{\mathbf{p}} - \mathbb{W}_s^f \left(\hat{V}_s \right) / \hat{V}_s$
Capacity W	$\mathbb{M}_s^d$ $\dot{\mathbb{M}}_s^d$	$m_W := \int_0^t \dot{m}_W(\tau) \, d\tau + m_W(0)$ $\dot{m}_W = \underline{\underline{\mathbf{F}}}_W \, \underline{\hat{\mathbf{m}}}$ $h_W := \rho^{-1} \, A_W^{-1} \, m_W$

Capacity A	$\mathbb{M}_s^d$ $\dot{\mathbb{M}}_s^d$	$m_A := \int_0^t \dot{m}_A(\tau)\, d\tau + m_A(0)$ $\dot{m}_A = \underline{\underline{\mathbf{F}}}_A\, \hat{\underline{\mathbf{m}}}$
Capacity A & W	$\mathbb{V}_{W+A}^d$	$0 = \dot{V}_W + \dot{V}_A$
Properties	$\hat{\mathbb{P}}_m$	$V_s := \rho^{-1}\, m_s$
Interfaces	$\mathbb{M}_s^e \quad 2,3,4,5,7$	$0 = \underline{\underline{\mathbf{F}}}_s\, \hat{\underline{\mathbf{m}}}$
Interfaces	$\mathbb{E}_s^e \quad 2,3,4,5,7$	$0 = \underline{\underline{\mathbf{F}}}_s\, \hat{\underline{\mathbf{w}}}^v = \hat{V}\, \underline{\underline{\mathbf{F}}}_s\, \underline{\mathbf{p}} = \underline{\underline{\mathbf{F}}}_s\, \underline{\mathbf{p}}$

The main feature here is that the level in the tank is a function of the slow part, namely the dynamic mass balance. Also the flow through the breathing pipe is determined by the dynamics in the tank. The dynamics of the water is given by the flows in and out, whilst the dynamics of the gas phase, the air, is driven by the change in the volume of the water in the tank and the fact that the total volume is constant. The capacity model applicable to P, J, O, P uses the mass balance for the same systems and the density.

4. Conclusions

The analysis of flow systems requires first a split into two separate descriptions for mass and mechanical energy. Whilst the mass balances are dynamic, the mechanical energy balances are event-dynamic assuming that the pressure propagates much faster than the level changes. Latter is used by implementing a singular perturbation assumption for all the systems or what in chemical engineering is usually referred to as pseudo-steady state.
The presented analysis can be further abstracted, which exploits the structural properties further, though it gets harder to communicate. Specifically, the depicted graph can be seen as a bipartite graph, with one set of nodes being the interfaces and the other being the capacities. The analysis shows that the fields appear as the driving forces for the transport in one half of the bipartite graph. The analysis though takes more space than we have available here, so we must leave this extension to a later exposition.
The fact that one requires the boundary conditions of the event-dynamic system to be defined seems quite obvious even though that is often a piece of intense discussion in practice.
How can these results be used? One of the main applications is in alarm and warning handling. Large plants suffer of alarm flooding and modern control systems are starting to do active alarm hiding by constructing alarm management systems (Hollender et al, 2007). Latter found some significant industrial interest for a good number of years, but has manifest itself clearly with the two patents (Sköld et al, 2010) and (Thurau, 2011). The apparent other application is Hazop analysis as documented in (Venkatasubramanian, 2000) and (Dunjóa, 2010).

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