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***Abstract* — This paper intend to extend the Multilevel Flow Modelling ontology by defining separation and conversion functions for representing mass balances in the physical systems such as process plant. Two modelling examples are provided in order to demonstrate how to use the two new mass flow functions and their causal roles in relation to other functions.**

Keywords* — *functional modelling, multilevel flow modelling, function ontology.

I. Introduction

Multilevel Flow Modelling (MFM) is applied to model the process plants in the perspective of the goals and functions. MFM ontology defines the concept of a function from several different perspectives. One of the aspects that an MFM function addresses is that a function can be viewed from both a static and a dynamic perspective. The static view of a function centers on the actors (roles i.e. commodity and components in the context of process plant) that are involved in realizing the function. The dynamic view of a function involves the actual actions those actors (roles) should perform.

The six basic MFM functions defined in the MFM ontology [1] can describe a relatively broad range of actions that are commonly applied in process plants: the material that flows through the system can be provided (represented by source functions), transported (represented by transport functions), stored (represented by storage functions), balanced (represented by balance functions), barred (represented by barrier functions), and discharged (represented by sink functions). The same actions can apply to the energy, which is normally carried by and exchanged between materials.

While this set of functions is adequate to represent the total mass and energy balances in a variety of process plants, they often fall short of representing some of the production goals that heavily rely on the properties of the material. For this reason, several ad hoc special functions have been used during the modelling practices such as in [2][3] to represent the detailed aspects of changes in material and its effect on the plant production and control goals. The special functions are named, following the nature of the property changes, as separation, mixing, distribution, and conversion. The names also comply with industrial convention.

The aim of this paper is to formally define and integrate two of the new functions mass separation and mass conversion into the existing MFM ontology with clear definition and causal rules. The definition and causal rules are introduced in Section 2. Two modelling examples, one for each function, are provided for demonstration purposes in Section 3. Section 4 offers discussions regarding MFM ontology extension and conclusions.

II. Mass Separation and Conversion

The authors assume that the readers already have obtained a basic understanding of MFM through a various selection of MFM literature such as [1], [4] and [5]. Here on forward, MFM terminology is used directly without further references.

A. MFM Flow Functions

The concept of a flow function defined in MFM ontology is in relation to its placement in the means-end structure (Fig.1). From the dynamic perspective, an action has to be performed for the function to be able to achieve an objective. Therefore, the roles that involved in an action has to be fulfilled so that the function can be realized. The most basic action roles are the agent that acts) and the object (that is acted upon) [5].

Take MFM mass transport function as an example (also illustrated in Fig.1), the function represents a stream of mass (object) that is transported. The agency of the transportation is provided by a combination of either the three possible sources: 1) the agency propagate from the mass flow's upstream or downstream through causal relations, 2) the agency propagate from other mass or energy flows though means-end relations, and 3) the agency is provided by a physical structure or component. All six MFM flow functions are defined in an analogous manner; such that causal reasoning rules can be systematically derived. Changes of the performance of the agents will influence the change of states in the objects.

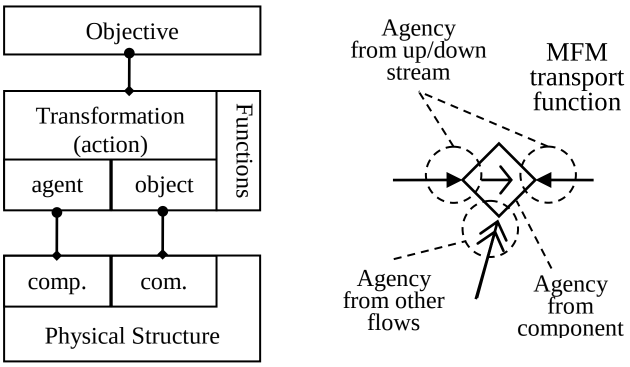

Fig. 1. Means-end structure and MFM mass transport function

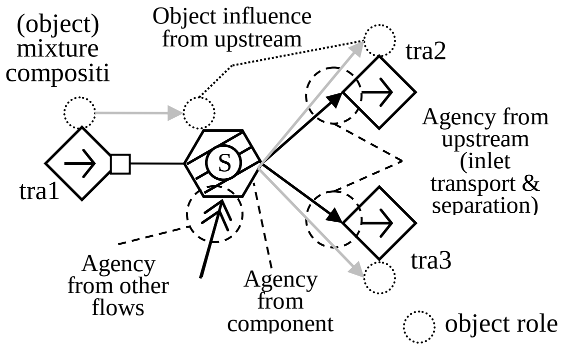

Fig. 2. Separation function and its connected transport functions

The observable realization of a function is the state of the object; naturally, this is used to evaluate the state of the function's performance. Since MFM model is a qualitative model, the function states are also qualitative states. For example, a transport function can have high flow rate or low flow rate comparing to its normal performance, and a storage function can have high level or low level states. Through the analysis depicted in Figure 1 above, the aspects to be considered when defining a MFM flow function can be summarized as follows: 1) the transformation (action) of the function.; 2) the object role and agent role of the function; 3)what model elements can provide the required agency; and 4) the states of the object. These four points are addressed in the following section when defining new MFM functions.

B. Mass Seperation Function

Separation processes, or processes that use physical, chemical, or electrical forces to isolate or concentrate selected constituents of a mixture, are essential to the chemical, petroleum refining, and materials processing industries [7]. MFM models can represent systems within the above-mentioned industries [2]. On an abstract level, the actions involved in a separation process can still be described by using the basic MFM balance, transport, and storage functions. In that case, the total mass balances between the mixture inlet and the total outlet of the separated streams are represented in the MFM model. However, the nature of the separation function itself is not represented specifically. To introduce the separation function, a similar analysis for MFM separation function as in the previous section is illustrated in Fig. 2.

The most significant difference between a separation and a normal MFM balance function is the requirement on the transformation of stream compositions during the separation, which means that there exist conditions for the materials to serve as object roles in the separation function, and also in its upstream and downstream transports.

The normal balance function has two causal signatures. One is to pass the agency from upstream to downstream or vice versa; the other is to balance different flow branches connected to its upstream or downstream. The separation function, in comparison, has only one upstream inlet flow. The total inflow and outflow are still balanced by the separation (the same as a balance function), but the distribution of flows after separation depend on: 1) the separation conditions, and 2) the composition of the flows through the separation (which is passed down from the inlet).

Draw from this analysis, the separation function can be defined in the same manner as other MFM flow functions.

Definition: *The (binary) mass separation function in MFM represents a system as a separator of two mass components. The function is characterized by a state variable indicating the quality of mass separation, the low quality means the purity of the downstream object is low. Note that only a low state is defined as an abnormal state. Each separation function can have one and only one upstream inflow, and at least two downstream outflows.*

The states of the object roles around separation functions are the key elements that will actually influence the process. The condition of the object roles has to be specified.

1) Upstream transport to a separation function has an object role that specify the condition of the mixture to be separated

2) The downstream transports from a separation function also have mixtures as objects, however, they should each has one predominate constituent compare to the upstream transport function.

Based on the definition and the specification of the object roles involved, causal reasoning rules can be defined as follows.

Firstly, MFM separation function should have the same across balance rules as normal balance functions. Secondly, a low amount of a certain component in the upstream transport functions' object role will cause a low flow to a certain transport function that represents this components dominant flow at the downstream side. Thirdly, MFM a separation function can be connected through means-end relation and producer-product relation as function target, the means function in this relation should contribute to the quality of the separation. Fourth, the quality of the separation influence the object role's purity state of the two downstream transports. All the influences are indicated in Fig.2.

C. Mass Conversion Function

Conversion function is firstly introduce to MFM model as energy conversion function and it is still being investigated by the author's research group. Conversion function can also apply to mass flow, where it indicates a chemical reaction. Chemical reaction engineering is a field of research of its own, however, since it is commonly used in the process plant, not only to produce chemical compound, but as briefly mentioned in the previous section, can also be used as means for separation.

By using the same analysis as in Fig. 1, we can define the MFM mass conversion function as follows:

Definition: *The mass conversion function in MFM represents the use of a system as a reactor of mass according to a specified stoichiometry. The function is characterized by a state variable indicating the rate of reaction; low reaction rate means the downstream object components state (product concentration) is low, and high reaction rate means the downstream object components state is low. Each separation function can have one or more upstream in flow(s), and one downstream out flow.*

Please note that chemical reactions may have multiple products; however, since the separation function has been defined in the previous section the reaction products can be separated further downstream.

Again, it is important to analyze the object roles around the mass conversion.

1) Upstream transport(s) to a mass conversion function has an object role that satisfy the condition of a reactant mixture.

2) The downstream transport(s) to a mass conversion has the reacted mixture as object, the reaction productshas to have an incresed concentration.

Based on the definition and the specification of the object roles involved, causal reasoning rules are defined for mass conversion as follows:

Firstly, a MFM mass conversion function should have the same causal reasoning rules as normal storage functions. Secondly, low flow of a limiting reactant will lead to a low product content in the downstream transport. Thirdly, mass conversion function can be connected through means-end relation producer-product as function target, the means function in this relation should contribute to the rate of the reaction (this can be catalyst, temperature or any other reaction condition). Fourthly, the rate of the reaction influences the downstream transport depending on whether it has an influencer relation to the downstream.

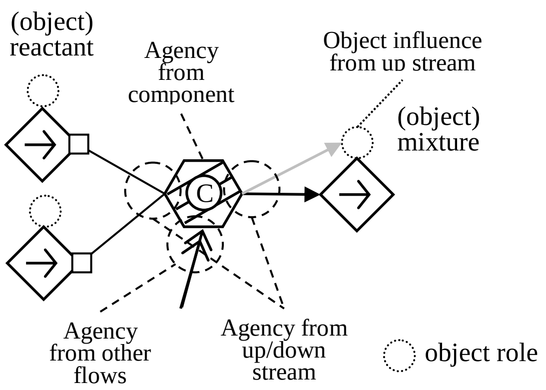

Fig. 3. Separation function and its connected transport functions

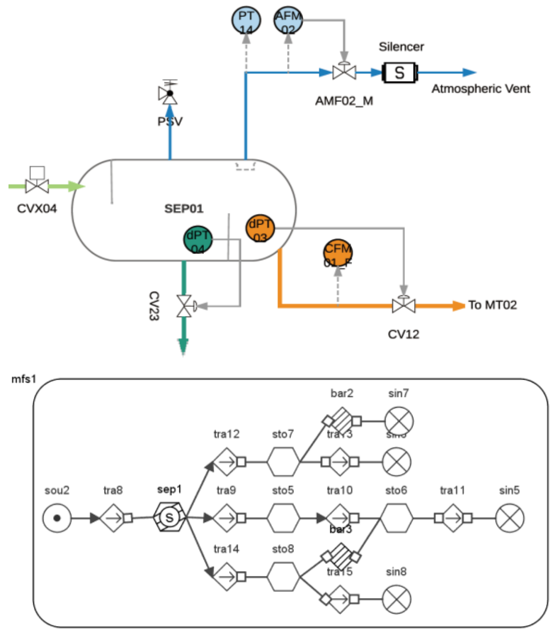

Fig. 4. Process flowsheet and mass flow structure for a three-phase separator.

III. Modeling Example

To demonstrate the usage of the mass separation and conversion functions, two modelling cases are presented in this section. The mass flow structure for a three-phase separator is presented for separation function, and the mass flow structure for a chemical deaeration process is presented to demonstrate the mass conversion function.

A. Three-phase Separator

The three-phase separator has been modeled by using MFM models in [6]. As the MFM function of separation was properly defined prior to this paper, the model presented here will be different from that show in [6]. The causal influences now can be describe more precisely. Due to the limitation of the paper, only a mass flow structure for the three-phase separator is presented. The pressure and temperature influences are not shown.

The system and the MFM model are shown in Fig. 4. Function sou2 represents the source of the mixture, function tra8 represents the inlet mixture, and sep1 is the separation function. The mass flow is separated into three different physical space within the separator: sto7 represent the gas storage on top of the separator tank, sto8 represent the water storage, sto5 represents the oil remained on top of the water chamber, and sto6 represents the oil stored in the oil chamber. Function tra3, tra11, tra15 and their downstream sink functions represent the gas, oil and water outlets respectively. Function bar2 represents the safety pressure valve that is closed during normal operation.

By using reasoning rules defined in Section II, we can analyze how changes in the composition of the mixture can lead to deviations in the downstream. For example, low level in sto6 indicates a low oil level. One of possible cause is low flow from the inlet tra8, another possible cause is a low oil content in the inlet mixture. In the two different scenarios, if the tra8 is low, then the water and gas inlet tra12 and tra14 are also low; if tra8 is normal, the oil content is low, then the water and gas inlet tra12 and tra14 should be higher than normal situation. In this way, it is possible to use a MFM model to identify abnormal states due to the property of the amterial components on top of the normal total mass balances.

B. Chemical Scavanger Deaeration Process

The second model subject is a chemical deaeration process. It is the final step for Oil and Gas platform injection water treatment. Both the system diagram and the MFM mass flow structures are shown in Fig. 5. In this process, the sea water is being treated by adding an oxygen scavenger to remove the remaining oxygen in the water. However, no separation is required after the reaction, so we can view the mass conversion function without a downstream separation.

In the MFM model, mass flow conversion represents the reaction between the scavenger and the dissolved oxygen. Function sou1 and tra1 represent the inlet of the dissolved oxygen in the sea water; function sou2 and tra5 represent the oxygen scavenger inlet.

Function tra3 and sin1 represent the outlet of the reaction product and remaining reactants leaving the system with the sea water discharge. The sea water mass flow represents the water flow. It mediates the transportation of the reactants and the product. The object roles for tra1, tra5, and tra2 are served by oxygen (reactant), oxygen scavenger (reactant), and mixture of the reactants and the produced chemical compound (all dissolved in the sea water).

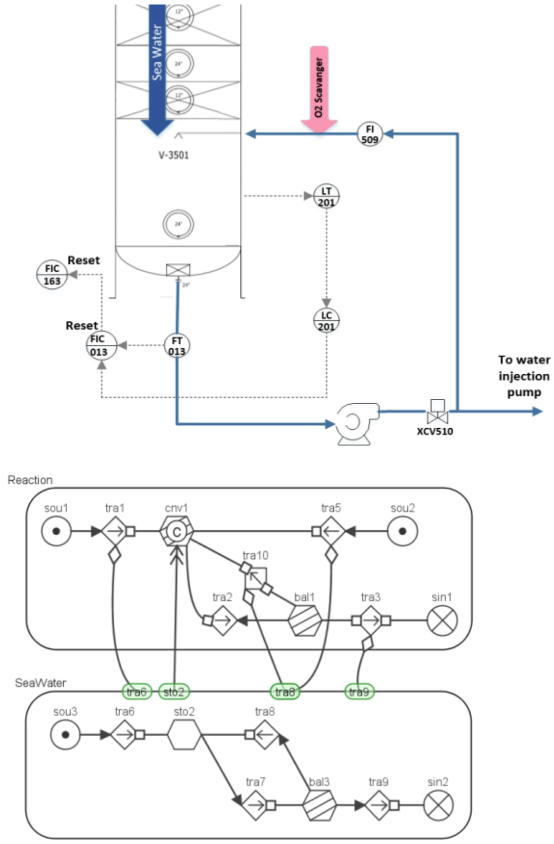

Fig. 5. Process Flowsheet and mass flow structure for a chamical deaeration.

Function tra10 and tra3 has the same object role as tra2 since no conversion or separation happens between those transports. The reactant flow rates will influence the state of the reaction, then it will further influence the state of the object role associated with tra2. A low level in the seawater flow will result in a longer reaction time, which will also influence the state of the reaction and the state of the object role in tra2.

IV. Discussion and Conclusions

This paper presented two examples of how MFM function ontology can be extended. Both the dynamic and static aspects of a function have to be taken into consideration. Even though the functions are defined mostly by the dynamic part, namely the transformation (action), the conditions for physical commodity or component to serve required action roles (the static view) are equally important. Only by analyzing the function roles, the causal relations between new functions and existing functions can be properly understood. The reaction process selected in this paper is very simple, which only involve two reactants. The reaction itself can happen without catalyst and the energy change caused by the reaction is also negligible. More modelling cases are required for finalizing the result from this paper. By using a similar analysis, more functions regarding change of the object role property can be defined. The already developed functions such as mass mixing, distribution, and energy conversion should be studied afterwards. The causal reasoning rules involving object roles has not been fully implemented in the DTU developed rule-based reasoning system. The work in this paper will be continued and tested by using models and data collected from real process systems.

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