Causality Validation of Multilevel Flow Modelling

Nielsen, Emil Krabbe; Gofuku, Akio; Zhang, Xinxin; Ravn, Ole; Lind, Morten

Published in:
Computers & Chemical Engineering

Link to article, DOI:
10.1016/j.compchemeng.2020.106944

Publication date:
2020

Document Version
Early version, also known as pre-print

Link back to DTU Orbit

Citation (APA):
https://doi.org/10.1016/j.compchemeng.2020.106944

General rights
Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.
Causality Validation of Multilevel Flow Modelling

Emil Krabbe Nielsen\textsuperscript{a,h,*}, Akio Gofuku\textsuperscript{c}, Xinxin Zhang\textsuperscript{a}, Ole Ravn\textsuperscript{a}, Morten Lind\textsuperscript{a}

\textsuperscript{a}Department of Electrical Engineering, Technical University of Denmark, Elektrovej 326, Kgs. Lyngby, 2800, Denmark
\textsuperscript{b}Department of Chemical Engineering, Technical University of Denmark, Saltofts Plads 227, Kgs. Lyngby, 2800, Denmark
\textsuperscript{c}Graduate School of Interdisciplinary Science and Engineering in Health Systems, Okayama University, 3-1-1, Tsushima-Naka, Kita-ku, Okayama, 700-8530 Japan

Abstract

Multilevel Flow Modeling is a methodology for inferring causes or effects of process system anomalies. A procedure for validating model causality is proposed, as interest has increased from industry in applications to safety-critical systems.

A series of controlled experiments are conducted as simulations in K-Spice, a dynamic process simulator, by manipulating actuators to analyse the response of process variables. The system causality is analysed stochastically under a defined range of randomly sampled process conditions. The causal influence of an actuator on a process variable is defined as a probability of a qualitative and discrete causal state.

By testing an MFM model, and interpreting the propagation paths produced by MFM, the results from MFM are compared to the stochastic causality analysis to determine the model accuracy. The method has been applied to a produced water treatment system for separation of liquid and gas, to revise the causal relations of the model.

Keywords: Causality, Multilevel Flow Modelling, Validation, Causal inference

1. Introduction

Multilevel Flow Modelling (MFM) provides an ontology for modelling the functions of process systems and relating them causally, to infer about causes for and effects of process anomalies \cite{1}. MFM models are built from the interpretation of design and operation related information such as diagrams, instructions and process knowledge from process experts. The model represents the functions of the system and the causal relations between them.

Applications of MFM models includes producing counter-action plans for bringing systems to a safe condition \cite{2}, risk assessments \cite{3,4}, diagnosis \cite{5,6}, alarm management \cite{7,8}, and process display design \cite{9,10}. Commonly modelled systems are nuclear power plants and oil and gas production systems. For such safety-critical systems it is of utmost importance that the system functions as intended, thus requiring
rigorous assessments and testing based on industry specific standards. Similar rigorous procedures should apply to models used for decision making related to the safety of safety-critical systems. For this reason, the work presented in this paper aims to provide a procedure for validating the causal relations of MFM models.

Previously the performance of only a few MFM models has been evaluated and no structured method has been proposed for such purposes. Most attention has been paid to this matter by Gofuku, although model evaluation has not been the primary purpose. The results from MFM models have been used to produce fault trees for risk assessment [11], fault diagnosis [12] and counter-action plans [13, 14] that have all been compared to expert opinions. In addition, a fault tree analysis (FTA) produced from MFM results has been compared to an FTA found in the literature of the same system [11, 12]. Counter-action plans derived from MFM results have been compared to results from dynamic process simulations [15]. Simulations have also been used as a reference to produce tables describing different failure modes that the MFM model could describe or classify correctly [4, 16]. The results produced by MFM, were proposed by Ming et al. [17] to be combined with an Artificial Neural Network for diagnosis. The ANN could either invalidate MFM inferences or elaborate on the inferences by MFM. To document the model maturity, meta-information was suggested by Heussen and Lind [18] to accompany models, which could very well be information from evaluation or validation processes.

A general and structured validation procedure has been proposed for validation of MFM models [19, 20]. However, the individual steps of the procedure lack in detail on how to apply it. In relation to this, a combined framework of an MFM model, a HAZOP and a dynamic process simulation were validated by Wu et al. [4]. Apart from this framework, other work included a comparison of MFM model results with information from a standard operation procedure [20]. Similar to Wu, the use of different methods for model validation was proposed by Yang et al. [21] to derive models for an Event-Tree, Goal Tree and Success Tree, Fault Tree and GO-FLOW from an MFM model. The models can then be used to indirectly validate the MFM model, by validating these models against other references. However, as validation was not the aim of the study, no details were introduced on model validation.

The structured approach proposed by Nielsen et al. [22] compares the results of MFM to those produced by experts, simulations or physical experiments. The approach is based on the principles proposed by Wu. An application of MFM for diagnosis introduced an example of how to evaluate the performance of MFM models for causal inference [5]. The validity of the causal relations of MFM models has only been addressed by Larsson et al. [23]. Larsson proposed the method multiple local property correlation for describing varying system causality from signal properties instead of the signal itself, as is the case for conventional correlation [24, 25]. The method was proposed for invalidating causal relations over time, as system behaviour would change.
In this study, we extend the previous work of Nielsen et al. [22] and Wu et al. [4] to a more complex model. The extension includes an interpretation of more than a single MFM propagation path, and a structured way of simulating tests to provide a reference for validation of causal relations in MFM models. In addition, a simple set of rules are proposed for revising an MFM model based on the validation results.

For validating models of system dynamics, Barlas [26] proposed an approach categorised into two stages dealing with structural validity and behavioural validity. To address structural validity either direct structure tests are proposed or structure-oriented behaviour tests. Structure-oriented behaviour tests are suggested rather than direct structure tests, as they are easier to formalise and quantify, and are qualitative and subjective to a lower degree. The purpose is to indirectly assess whether a model structure is valid, by applying behaviour tests to both the model and simulation. Suggested tests include extreme testing, behaviour sensitivity and a combination of both Barlas [26].

An example of combining extreme testing and behaviour sensitivity is Qualitative Feature Analysis, in which qualitative features of the system behaviour are compared to the qualitative features of the model output [27]. Multilevel Flow Modelling is a method for causal inference. The method provides an ontology for graphically formulating knowledge of process systems such that models can be used for causal inferences. The validity of the pre-requisite conditions of knowledge-based models has generally lacked quantification according to Wise et al. [28] thereby resulting in uncertainty. Moreover the choice of validation tests must be representative of model applications and be sufficiently sensitive to detect errors. Thus Wise et al. [28] argues that the tests must cover the intended conditions of the model application, rendering a sole application of extreme testing unfit, despite being likely to overcome the issue of performing sufficiently sensitive tests.

A common approach to address uncertainty is to include it as a part of the tests of model validation, which is a common requirement of governmental agencies for models related to decision making processes on health, environment [29] or safety-related issues. As causal relations of MFM models are based on the knowledge of process designers and experts, and the interpretation of available formal descriptions of the process system and its operation, no probabilities are included for these being correct. The process conditions for which causal relations are assumed valid are not explicitly expressed for MFM models. As MFM models are based on knowledge, imprecise specifications of the process conditions introduce uncertainty. This type of uncertainty is referred to as subjective risk. In addition, the magnitude required for causes to produce an effect is unknown, and most likely varies with the process conditions.

Conventional methods for analysing causal relations are listed by Yu and Yang [30] and include Granger causality, extended Granger causality, nearest neighbour methods, cross-correlation and transfer entropy. The aforementioned methods are commonly applied to historical and surrogate data to analyse the system
The work presented here aims to provide a structured method for validation of causality in MFM models based on a stochastic approach to perform behaviour-oriented structure tests by simulating controlled experiments. The simulation inputs are a set of process conditions and an actuator step change. Uncertainty is imposed on the input to analyse the output probabilistically. Change detection is used to determine the change of effects in percentage, and by comparing the change to a set of thresholds, the output is converted to causal states that describe the most probable causal influence. The output of the analysis is formulated into a single qualitative state and the probability of that state for the sampled simulation input. The work presented here is based on the method for stochastic causal analysis and the results of the analysis presented by Nielsen et al. [31].

The method is first explained for a simple and theoretical example and then applied to an MFM model of a Produced Water Treatment system, based on which a set of simple rules are proposed for revising the causal relations. These rules are then used to improve the coherence between the analysed causality and the MFM model causality.

2. Multilevel Flow Modelling

Multilevel Flow Modelling is a functional modelling ontology for expressing a system’s functionality and causal dependencies. MFM models are causal graphs, that explain the causal relationship between different functions and objectives. The functions are ordered in a hierarchical means-end abstraction according to how functions realise objectives and other functions. The models can be used for rule-based inference on causes for anomalies of system operation. Similarly, inferences can explain effects an anomaly.

In the following, the term flow function will be used for referring to an MFM primitive, an object of the ontology used for modelling, and the term function to functionality of a process system. The MFM ontology includes a defined set of function primitives, which are qualitative and discrete representations of physical mechanisms [32]. The functions of the process system are modelled using the flow functions of the MFM ontology.

In general, two different causal relations are distinguished between; an influencer which is a causal relation that can affect both directions, and a participant relation that can only affect in one direction. Other causal relations, the means-end relations, are similar causal implementations of the participant relation but have distinct descriptive meanings. The influencer relation represents causal symmetry, such that a flow function $A$ can be a cause of flow function $B$ written as: $A \rightarrow B$, and the opposite $B \rightarrow A$. The participant relation represents causal asymmetry such that $A$ can be a cause of $B$: $A \rightarrow B$, but $B$ cannot be a cause of $A$: $B \not\rightarrow A$. The notation of MFM ontology denotes symmetric causality as $\rightarrow$ and asymmetric causality as
One challenge of using MFM is to determine whether a causal relation should exist between two flow functions and whether it is an influencer or a participant relation. Reasons for this are; causal relations of the models are implicitly conditional on specific process conditions. Other causal relations of the model may provide incorrect causal results for those process conditions, as they have been modelled conditional on a different set of implicitly defined process conditions. Causal relations of the model may thus be based on different assumptions for which process conditions they are valid. Other reasons involve the inherent bias towards causal asymmetry in subjective judgements of causality [33], as MFM models are constructed based on both objective and inter-subjective knowledge of process systems as argued by Wu et al. [19].

We propose a method for validating the causal relations of MFM models, to provide an objective and quantitative reference for the selection of causal relations. The proposed method only analyses the compound causality, which is the combination of direct and indirect causality. For this reason, the method cannot account for causal paths, but merely the compound causality from an actuator to process variables. The majority of causal analysis methods only identify compound causality. However, multivariate approaches exist for analysing either direct or indirect causality [34]. The process flow from P&IDs is used for capturing causal paths by Yang et al. [35], for comparison with compound causality analysed with Transfer Entropy. Compound causality can however not address spurious causality. Sensitivity analysis can however address the issue of spurious causality for the proposed method [31]. Flow functions will be referred to in the following way (Flow structure name):(Flow function name):(Flow function type):(State). If referring to the flow function in general the (state) will be omitted.

3. Validation methodology

The method for validating MFM causality is shown in fig. 1. It can be categorised into four parts: analysing system causality, testing MFM causality, result comparison and model revision. At first, all actuators for testing are defined in both the MFM model and the simulation. Tests are then sampled based on a defined uncertainty for an actuator step change (the cause) and estimated process conditions. These samples are evaluated in numerical simulations by using K-Spice. The output of the simulations is time series of process variables, that are converted to qualitative states. The MFM model is tested by inferring effects of state changes to the flow functions associated with manipulable actuators. The qualitative states from the causal analysis of the simulations and the MFM inferences are compared to determine how well the results correspond. Lastly, the MFM model is revised based on the accuracy of different model parts.
Figure 1: Procedure for testing the MFM model and the simulations for causality comparison.
3.1. Causal analysis of simulations

The method used for analysing the causality of the system consists of four simple steps Nielsen et al. [31]: probabilistic experimental design, simulation, change detection and qualitative state conversion. For notational simplicity, the procedure is described for the case of only a single actuator. As the causality of MFM models is implicitly defined over a range of process conditions, the simulations are evaluated over this range. In the first step, a set of \( M \) process conditions, including the actuator step change, are sampled randomly with Latin Hypercube Sampling (LHS) into \( N \) samples in unit hyperspace. The samples are then converted to real process values by the inverse cumulative distribution functions defined by a mean and a standard deviation. The mean and standard deviation are estimated as representative for the process conditions of the system for which the MFM model will be assumed valid. Given little is known about the exact relationship between actuators and the process variables, the actuator step change is varied with equal probability over the entire range of operation from fully open to fully closed; defined by an inverse cumulative uniform distribution function. The process conditions are sampled as the input variables \( X_{m,i} = [X_{1,i}, X_{2,i}, ..., X_{M,i}] \) for \( i = [1, 2, ..., N] \) simulations and \( m = [1, 2, ..., M] \) process conditions.

The sampled input variable \( X_{m,i} \) is evaluated as numerical simulations in K-Spice such that an output \( Y_i = f(X_i) \) is obtained for every sample \( i \). This output \( Y_{i,j,k} \) for \( k = [1, 2, ..., K] \) is a time series of \( K \) samples for the \( j = [1, 2, ..., J] \) process variables. First the process conditions \( X_{m,i} \) for \( m < M \) are loaded at the beginning of every simulation and kept constant. Next, the simulation runs for the duration of \( t_1 \) to reach stable operation, defined by the following three conditions:

\[
\begin{align*}
  \frac{dm_{in}}{dt} &\approx 0, \\
  \frac{dm_{out}}{dt} &\approx 0 \\
  m_{in} &\approx m_{out}
\end{align*}
\]

for \( m_{in} \) being the inflow of mass to the system, and \( m_{out} \) the outflow of mass. The mass and energy balances should thus hold as a condition for a stable system. At time \( t_1 \), the step change \( X_{m,i} \) for \( m = M \), is introduced to the actuator control signal which remains constant for that actuator for the remaining time \( t_2 \) of the simulation. The step change is denoted as \( \alpha \), and the step response of process signals as \( \beta \). The response \( \beta \) is the effect size, which is the magnitude of the effect. The direction of the effect is given by the sign of \( \beta \).

A section \( y_{i,j,k} \) of the time series \( Y_{i,j,k} \) is selected based on a time interval defined from \( t_s \) seconds before the actuator step change, at \( t_1 \), until \( t_e \) seconds after the step change. Change detection is used to determine a sample in time of \( y_{i,j,k} \) where the mean of the selected time series \( E[y_{i,j,k}] \) changes abruptly. The same method for change detection is applied as in [22]. The step response, which is the change in mean \( \beta_{i,j} \) of \( y_{i,j,k} \), is compared to a lower and upper threshold that defines whether the effect size is considered to be significantly large for a causal relationship to exist between the actuator (cause) and the process variable (effect).

The response \( \beta_{i,j} \) of every time series is classified as a qualitative state \( S_{i,j} \) based on the thresholds. The
states low, normal and high are represented numerically as \( S_{i,j} = \{-1, 0, +1\} \) and can be determined as:

\[
S_{i,j}(\beta) =
\begin{cases} 
-1, & \text{if } \beta < L_{\text{low}} \\
0, & \text{if } L_{\text{low}} \leq \beta \leq L_{\text{high}} \\
+1, & \text{if } L_{\text{high}} < \beta 
\end{cases}
\]  

(1)

A single state \( \bar{S}_j^+ \) is determined for every process variable, associated with a probability for the process variable to attain the given state. The probability is determined as the probability of the process variable attaining a given state, conditioned on the actuator state and the process conditions. Thus, both the change in mean \( \beta_{i,j} \) of the process variable and the actuator step change \( \alpha_{i,j} \) are compared to the lower and upper thresholds \( L_{\text{low}} \) and \( L_{\text{high}} \). As the states are mutually exclusive, the state \( \bar{S}_j^+ \) is then determined as:

\[
\bar{S}_j^+ =
\begin{cases} 
\text{low,} & \text{if } P(S_j = -1 | \alpha = +1, H) > P(S_j = 0 \cup S_j = +1 | \alpha = +1, H) \\
\text{normal,} & \text{if } P(S_j = 0 | \alpha = +1, H) \geq P(S_j = -1 \cup S_j = +1 | \alpha = +1, H) \\
\text{high,} & \text{if } P(S_j = +1 | \alpha = +1, H) > P(S_j = 0 \cup S_j = -1 | \alpha = +1, H) 
\end{cases}
\] 

(2)

A single state \( \bar{S}_j \) is selected to represent the causal relation between a process variable and an actuator for the tested process conditions. The state \( \bar{S}_j \) is the most probable state conditioned on the actuator state. In this work, the state \( \bar{S}_j \) is only presented conditional on the actuator state high (\( \alpha = +1 \)) denoted as \( \bar{S}_j^+ \).

A qualitative trend table (QTT) introduced in [22] is comprised of those states that represent the particular process variables conditioned on a particular state of an actuator. The QTT is thus an asymmetrical description of causality between an actuator and a process variable. It describes whether the process variables are causally dependent or independent of an actuator. In addition, it describes the causal dependence as an influence on the process variable as being either positive or negative. The QTT should contain results for all actuators and preferably also boundary conditions.

Causal relations in MFM are qualitatively proportional [35]. Therefore, the QTT can be defined by only representing causes described by either a high \( \bar{S}_j^+ \) or a low \( \bar{S}_j^- \) state of the actuators, and not necessarily both. In this study, only the high actuator states are presented. The qualitative proportionalities can be expressed in the following way for the flow functions \( A \) and \( B \) and a corresponding state:

\[
\begin{align*}
A: \text{high} \rightarrow B: \text{low} & \iff A: \text{low} \rightarrow B: \text{high} \\
A: \text{high} \rightarrow B: \text{high} & \iff A: \text{low} \rightarrow B: \text{low}
\end{align*}
\]

The actuator state high can be substituted in eq. (2) for a low actuator state, to determine a single state \( \bar{S}_j^- \) that represents the most probable response of \( \beta_{i,j} \) conditioned on a low actuator state.

### 3.2. Testing MFM causality

When testing the causality of MFM models, all flow functions should ideally be tested to determine how well the results represent the behaviour of the physical system. Not all flow functions do however have a basis
for comparison. Nor may it be meaningful to test all flow functions. For complex knowledge-based systems, O’leary [37] argued that only highly certain or risk-related knowledge should be tested. The following two rules are proposed to guide the modeller in testing:

- Any flow function expected to be used as an input to the model should be tested.
- Any flow function expected to be used as an output from the model should be compared.

MFM models are typically used for explaining what caused a deviation of the system, and what the effects could be. In this case, the input would be a state of a process variable or a sensor. Process variables (sensors) cannot be directly changed or manipulated via controlled experiments. It is not possible to increase the pressure of the separator, without changing the condition of something else. However, approaches exist in modern mediation analysis for introducing estimated changes to indirect effects [38].

Physical equations or laws allow for such changes. The ideal gas law is formulated as $PV = nRT$, where $P$ is the pressure, $V$ is the volume, $n$ is the amount of gas in mol, $R$ is the ideal gas constant and $T$ is the absolute temperature. The ideal gas law allows for changing process variables while keeping others constant, such as the amount of gas, to determine the effects on the pressure, temperature and volume. This is however not meaningful, as somethings need to cause this change, and dependent on the cause, various conditions may apply that contradict the conditions. Doing this would determine the causal relationship deterministically under the assumptions that anything else is constant.

The state of flow functions in MFM can be changed to introduce system deviations. MFM can then be used for analysing the effects of the deviation. An actuator can be manipulated in MFM models, by changing the state of the flow function associated with the actuator in order to analyse the effects. Actuators can be physically manipulated to analyse the response of process variables. The same test can thereby be carried out in an MFM model, and a physical system. As physical tests may compromise the safety of systems, we propose to use dynamic simulations to produce a basis for comparison of the inference results form MFM.

The model boundaries are defined by the sources and sinks in an MFM model. When the system is stable, no mass or energy accumulates in the system. It should thus be possible to test the system, by changing the boundary conditions. The boundary conditions can be manipulated in the model, but also on a physical system or in simulations, as the system will be connected to something upstream and downstream. Therefore, the systems outside of the boundary can be manipulated, to test the boundaries of the MFM model.

Boundary conditions of MFM models and flow functions associated with actuators can be manipulated and should thus be used to test the model. Then, by testing the boundary conditions or the actuators $\alpha$ it is possible to determine if they are causes of the effects $\beta$. As the effect $\beta$ cannot be manipulated, $\beta$ is assumed valid for all paths between where the actuator $\alpha$ propagates to or through $\beta$. MFM has the capability of
inferring about either causes or effects. It is therefore assumed that if \( \beta \) is inferred as an effect of \( \alpha \), and the inference is valid, then inferring that \( \alpha \) is the cause of \( \beta \), is also a valid inference. Thus, if the deductive inferences are valid, then the deductive inferences are assumed valid.

When inferring about causes or effects, the propagations may include flow functions that have not been validated by comparison to a reference such as simulations. It is assumed that if a flow function is on a path between two flow functions that have been validated, that flow function is regarded as valid if no junctions exist on that path. Otherwise, it is regarded as untested. The validation of causal relations of MFM models should explicitly state what has been part of the validation, and what has not been. As not all parts of the model can be validated in practice with the proposed approach, other methods should be used for the remaining parts.

3.3. Example of MFM model testing

A system of two tanks is used as a theoretical example to explain the interpretation of propagation paths. The MFM model of the system is shown in fig. 2. The sensors Q1, Q2 and Q3 are flow rate sensors. Water is fed to a tank with the water level measured by the sensor h1. The tank has two outlets. One outlet leads to an additional tank, and the other to the output of the system. A control valve CV at the outlet of the first tank controls the water level h2 of the second tank, and thus indirectly the level of h1. The second tank has an outlet, which mixes with the output of the first tank. The actuator, being the control valve, has been tested in MFM to produce propagation paths. The sequence of these paths are:

\[
\begin{align*}
\text{mfs:CV:tra:high} & \rightarrow \text{mfs:h1:sto:low} \rightarrow \text{mfs:Q1:tra:high} \\
\text{mfs:CV:tra:high} & \rightarrow \text{mfs:Q2:tra:low} \rightarrow \text{mfs:h2:sto:high} \rightarrow \text{mfs:tra:tra:low} \\
& \rightarrow \text{mfs:h1:sto:high} \rightarrow \text{mfs:Q1:tra:low}
\end{align*}
\]

Associations between actuators and flow functions, and sensors (process variables) and flow functions should be explicitly defined. Once this association has been established the results from the analysis of the
simulations can be compared to the results from testing the MFM model. A qualitative trend table (QTT) is produced based on the results from flow functions associated with sensors and actuators. In this example, two propagation paths are produced from one actuator flow function. Each path in eqs. (3) and (4) is represented as a row in the QTT. The columns describe the sensor’s response in each path. All flow functions associated with sensors should be present as individual columns in the QTT, with the first column being the actuator. All flow functions present in the propagation paths that are not associated with components are omitted from the QTT. In the above example, the flow function mfs:tra:tra has no association to a component, and can thus not be validated by the simulation. For this reason, flow functions with no association are not included in the QTT in table 1. The states of the flow functions in the paths are represented by \( + \) for a high state with a red colour, a blue colour \( - \) for a low state and a grey colour \( 0 \) for neither a high nor a low state propagation. Thus, as mfs:Q3:tra is not an effect of mfs:CV:tra in either of the two propagation paths, the sensor is assigned the grey colour \( 0 \) for both paths. This procedure is repeated for all actuators.

<table>
<thead>
<tr>
<th></th>
<th>h1</th>
<th>h2</th>
<th>Q1</th>
<th>Q2</th>
<th>Q3</th>
</tr>
</thead>
<tbody>
<tr>
<td>CV-1</td>
<td>-</td>
<td>-</td>
<td>0</td>
<td>+</td>
<td>0</td>
</tr>
<tr>
<td>CV-2</td>
<td>+</td>
<td>+</td>
<td>-</td>
<td>-</td>
<td>0</td>
</tr>
</tbody>
</table>

3.4. Comparison of causality

In this step, each propagation path from MFM is compared to the set of uniquely defined causal relations from the causal analysis of the simulations. The previously introduced case by Nielsen et al. [22] provides metrics of the similarity between results from testing an MFM model and a validation set. The presented model is simple and produces no propagation paths that contradict each other. In the following, the approach from the simple case of a single propagation path is extended to the case of multiple contradictory propagation paths. The following set of rules for the comparison of propagation paths to a validation set are proposed:

- Any contradictive states between the validation set and the MFM results are undesired, unless the modeller or process expert, can provide sense to the result.
- A minimum of one propagation path needs to include the results from the simulations.
- In relation to the above; a normal state is acceptable, as long as one path includes the result of the simulation.
- Contradictive propagation paths are unwanted, unless the modeller or process expert, can provide sense to the result.

The results from the QTT from MFM and from the simulations are combined into a single table. The results from the simulations are used as a validation set. The validation set is a matrix denoted as \( V_{j,q} \).
for $q = [1, 2, ..., Q]$ actuators and for $j = [1, 2, ..., J]$ process variables, with $Q$ denoting the total number of actuators and $J$ the total number of process variables. The result from MFM is a matrix denoted as $F_{j,q,r}$ for $r = [1, 2, ..., R]$ propagation paths with $R$ denoting the total number of paths. The entries from the results are shown in table 2.

The process conditions have been sampled and evaluated in 50 simulations of the two tank example shown in fig. 2. The result from applying the method for conversion of simulation outputs to qualitative states are shown in the first row of table 2. Similarly, the results from the MFM inferences shown in table 1 are shown in the rows below the validation row in table 2.

When a propagation from MFM does not affect a specific process variable, it is proposed to treat it as the state normal illustrated by a grey colour, indicating no effect. When evidence exists of no relation is used, whereas is used when no evidence exists of a relation between a cause and an effect, and neither does any evidence of a relation exists. Therefore and are considered to explain the same omission of a causal effect, causal independence, thus the flow function’s state is normal.

<table>
<thead>
<tr>
<th>Table 2: Example of comparison of the QTT from simulations and the QTT from MFM with matrix notation.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Simulations</td>
</tr>
<tr>
<td>----------------------------------</td>
</tr>
<tr>
<td>CV</td>
</tr>
<tr>
<td>Propagation path 1</td>
</tr>
<tr>
<td>Propagation path 2</td>
</tr>
</tbody>
</table>

The results from all propagation paths that correspond to a particular actuator are converted into a single value by using the accuracy metric for binary prediction. The metric accounts for the ratio between correct (true) and incorrect (false) predictions of a given process variable and a given actuator. The accuracy is calculated based on a set of predicted observations represented by the propagation paths from MFM, and a validation set considered as actual observations. All predictions are compared to the observations to construct a confusion matrix that describes the true, and the false predictions used to determine the accuracy:

\[
\text{Accuracy} = \frac{\text{Correct predictions}}{\text{All predictions}} \tag{5}
\]

A low accuracy indicates a low correspondence of the results with a value of 0 being the lowest, and a value of 1 being the highest for equal results. The states of $F_{j,q,r}$ are all classified as either true (1) or false (0) in the matrix $C_{j,q,r}$ for $j = [1, 2, ..., J]$, $q = [1, 2, ..., Q]$ and $r = [1, 2, ..., R]$. Predictions are considered as true or false dependent on the state of the actual observation:

Given the actual observation of process variable $j$ for actuator $q$ in $V$ is a normal state, then the states of the predictions of process variable $j$ for actuator $q$ from $F$ are classified as follows: a
normal state is a true prediction, and either a high or low state is false. This can be formulated as logical conditions:

\[
C_{j,q,r} = \begin{cases} 
0 & \text{if } V_{j,q} = \text{normal} \land (F_{j,q,r} = \text{low} \lor F_{j,q,r} = \text{high}) \\
1 & \text{if } V_{j,q} = \text{normal} \land F_{j,q,r} = \text{normal} 
\end{cases} \tag{6}
\]

Given the state of the actual observation \( V \) is high, the states of the predictions \( F \) are classified as follows: a high state is true, a low state is false, and only if no high state is present in the predictions of process variable \( j \) for all propagation paths \( r \), a normal state is considered as false. This can be formulated as logical conditions:

\[
C_{j,q,r} = \begin{cases} 
0 & \text{if } V_{j,q} = \text{high} \land F_{j,q,r} = \text{low} \\
0 & \text{if } V_{j,q} = \text{high} \land F_{j,q,r} = \text{normal} \land (F_{j,q,r} = \text{high} \lor \exists r \in \mathbb{N}) \\
1 & \text{if } V_{j,q} = \text{high} \land F_{j,q,r} = \text{high} \\
1 & \text{if } V_{j,q} = \text{high} \land F_{j,q,r} = \text{normal} \land (F_{j,q,r} = \text{high} \lor \exists r \in \mathbb{N}) 
\end{cases} \tag{7}
\]

Given the state of the actual observation \( V \) is low, the states of the predictions \( F \) are classified as follows: a low state is true, a high state is false, and only if no high or low state is present in the predictions of process variable \( j \) for all propagation paths \( r \), then a normal state is considered as false. This can be formulated as logical conditions:

\[
C_{j,q,r} = \begin{cases} 
0 & \text{if } V_{j,q} = \text{low} \land F_{j,q,r} = \text{high} \\
0 & \text{if } V_{j,q} = \text{low} \land F_{j,q,r} = \text{normal} \land (F_{j,q,r} = \text{low} \lor \exists r \in \mathbb{N}) \\
1 & \text{if } V_{j,q} = \text{low} \land F_{j,q,r} = \text{low} \\
1 & \text{if } V_{j,q} = \text{low} \land F_{j,q,r} = \text{normal} \land (F_{j,q,r} = \text{low} \lor \exists r \in \mathbb{N}) 
\end{cases} \tag{8}
\]

The resulting matrix \( C_{j,q,r} \) for the example in table 2 thus becomes:

\[
C_{j,q,r} = \begin{bmatrix}
C_{1,1,1} & C_{2,1,1} & C_{3,1,1} & C_{4,1,1} & C_{5,1,1} \\
C_{1,1,2} & C_{2,1,2} & C_{3,1,2} & C_{4,1,2} & C_{5,1,2}
\end{bmatrix} = \begin{bmatrix}
1 & 0 & 1 & 1 & 0 \\
0 & 0 & 0 & 1 & 0
\end{bmatrix} \tag{9}
\]

The first and second condition of eq. (5) applies as no propagation path of variable h2 contains a low state. Therefore, \( C_{2,1,1} = 0 \) and \( C_{2,1,2} = 0 \). At least one propagation path contains a true prediction for the variable Q2. Therefore, the fourth condition of eq. (5) applies to \( F_{4,1,1} \), and thus \( C_{4,1,1} = 1 \). No propagation path contains any true prediction for the variable Q3. Therefore the second condition of eq. (7) applies and thus \( C_{5,1,1} = 1, C_{5,1,2} = 1 \).

The accuracy can be calculated when all inferences are classified as either true or false. The classification of all propagation paths \( r \) belonging to actuator \( q \) are then used to calculate the accuracy of every process
variable $j$:

$$A_{j,q} = \frac{\sum_{r=1}^{R} C_{j,q,r}}{R}$$ (10)

This is repeated for every actuator. The mean accuracy of each actuator $\bar{A}_q$, and each process variable $\bar{A}_j$ can then be calculated as:

$$\bar{A}_j = \frac{\sum_{q=1}^{Q} A_{j,q}}{Q}$$ (11)  \hspace{1cm} $$\bar{A}_q = \frac{\sum_{j=1}^{J} A_{j,q}}{J}$$ (12)

The mean accuracy of actuator $q$ is calculated as the mean of the accuracy of all $J$ process variables for actuator $q$. Similarly, the mean accuracy of process variable $j$ is the mean of the accuracy of process variable $j$ for all $Q$ actuators. Lastly, a single metric can be provided for the entire MFM model, as the mean accuracy of all combinations of $Q$ actuators and $J$ process variables:

$$\bar{A} = \frac{\sum_{j=1}^{J} \sum_{q=1}^{Q} A_{j,q}}{JQ}$$ (13)

The accuracy of the classifications in table 2 can be represented as shown in table 3. The results of $\bar{A}_{j,q}$ are identical to $\bar{A}_j$, and $\bar{A}_q$ is identical to $\bar{A}$ as this case only includes a single actuator.

Table 3: Model $\bar{A}$, actuator $\bar{A}_q$ and process variable $\bar{A}_j$ accuracy.

<table>
<thead>
<tr>
<th></th>
<th>h1</th>
<th>h2</th>
<th>Q1</th>
<th>Q2</th>
<th>Q3</th>
<th>$\bar{A}_q$</th>
</tr>
</thead>
<tbody>
<tr>
<td>CV</td>
<td>0.5</td>
<td>0</td>
<td>0.5</td>
<td>1</td>
<td>0</td>
<td>0.4</td>
</tr>
</tbody>
</table>

$$\bar{A}_j = 0.5 \hspace{1cm} \bar{A}_j = 0.5 \hspace{1cm} \bar{A} = 0.4$$

3.5. Revision of causal relations

The aim of revising the causal relations is to improve the accuracy of the MFM model. As argued by Wise et al. [28], validation should not be a process carried out after modelling but both should be carried out iteratively. The evaluations thereby aid the modeller in decisions for improving the model validity to converge as a cumulative process towards a specified requirement. The accuracy from eqs. (11) to (13) are metrics that can provide information about the convergence towards a specified requirement. A straight forward approach would be to start with either the process variables or the actuators with the lowest accuracy. To revise the causality, the following actions have been identified:

- An influencer relation can be substituted for a participant relation, to limit the cause from propagating further to avoid high or low states.
• A participant relation can be substituted for an influence relation, to *allow* the cause to propagate further to produce high or low states.

• A means-end relation can be inserted to *allow* the cause to propagate further to produce high or low states.

• A means-end relation can be removed to *limit* the cause from propagating further to avoid high or low states.

• A means-end relation can be moved from one flow function type to a different flow function type to change the propagated state from high or low to the opposite state.

• A diverging (splitting) flow function can be inserted to introduce an *upstream* effect propagation of the opposite state and removed to avoid it.

• A converging (merging) flow function can be inserted to introduce a *downstream* effect propagation of the opposite state and removed to avoid it.

The above-listed actions can be used for revising the model to do the following: limit propagation from flow functions, allow propagation to flow functions or introduce a different state to propagations of flow functions. However as MFM models are functional representations of the physical system, the model should not be revised without keeping the functionality and structure of the physical system in mind.

As model complexity increases,

Changing a relation for one actuator may influence the result of other actuators. The method, therefore, becomes a compromise between what behaviour is prioritised. It is, however, important to identify such compromises as they represent limitations of the model, which will inherently influence the model application. The need for compromising model accuracy becomes more prominent as model complexity increases.

For the previously introduced example, the process variables with the lowest accuracy are h2 and Q3. The flow function mfs:CV:tra:high should propagate as mfs:h2:sto:low and not as a high state. The propagation path of eq. (4) first propagates downstream to a converging flow function and then upstream.

The influencer relation of the converging flow functions mfs:bal:bal → mfs:Q2:tra can thus be substituted for a participant relation, to limit the propagation from propagating upstream. However, only the path from eq. (4) is then produced. Thus, the participant relation between the flow functions mfs:h1:sto —— mfs:tra:tra can be substituted for an influencer relation. To produce a high state for Q3, the participant relation between mfs:bal:bal —— mfs:Q3:tra can be substituted for an influencer relation. However, this enables the flow function mfs:CV:tra to propagate to mfs:Q3:tra both upstream and downstream, thereby producing either a low or a high state. To avoid this, a storage or balance flow function must be introduced in combination with a transport flow function between mfs:bal:bal —— mfs:Q2:tra. Two participant relations must be present in this path to avoid propagations from mfs:Q2:tra to mfs:Q3:tra. However, this means, that the water level h2 can only influence the total output of Q3 through the water level of h1. These model revisions produce the results shown in table 4. According to the previously introduced method for
calculating $\hat{A}$, the resulting accuracy is $\hat{A} = 1$ for the revised model.

### Table 4: Comparison of the revised model example to the simulations.

<table>
<thead>
<tr>
<th></th>
<th>h1</th>
<th>h2</th>
<th>Q1</th>
<th>Q2</th>
<th>Q3</th>
</tr>
</thead>
<tbody>
<tr>
<td>CV</td>
<td>-</td>
<td>-</td>
<td>+</td>
<td>-</td>
<td>+</td>
</tr>
<tr>
<td>CV-1</td>
<td>-</td>
<td>0</td>
<td>+</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>CV-2</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>+</td>
</tr>
<tr>
<td>CV-3</td>
<td>-</td>
<td>-</td>
<td>0</td>
<td>-</td>
<td>0</td>
</tr>
</tbody>
</table>

4. MFM model of system

The proposed method is applied to a dynamic process simulation and an MFM model of a produced water treatment system for high pressure separation. A multiphase composition of gas, oil and water is fed to the system from subsea wells. The system separates the mixed composition into a liquid and a gas stream. The gas is fed to a subsequent gas production system, and the oil and water is fed to a subsequent low pressure separation system. The MFM model of the system is shown in fig. 3 and the P&ID from K-Spice in fig. B.5 in Appendix B. The functions are named according to the sensor names and/or the actuator they are associated with. Functions shown in blue are functions associated with sensors. The mappings between flow functions and the system components can be found in Appendix A.

The main objective of the system is to separate water, oil and gas in a gravity separator. The separator consists of a feed side chamber and an oil side chamber that are separated by a wall. On the feed side, the water flows to the bottom of the separator, and the oil flows on top of the water. By maintaining the level of the multiphase feed of oil and water, the oil flows over the separator wall, and the water flows through an outlet at the bottom of the separator. The objective of maintaining the water level, $WLvlNormal:obj$, is realised by the water level control, that maintains the level on the feed side, by restricting or enabling water to flow through the control valve mfs:Q3CV1:tra at the water outlet on the feed side.

The objective $OilLvlNormal:obj$ ensures that the flow of oil from the feed side to the oil side is possible, thus enabling separation. In addition, it supports maintaining the pressure in the separator. This objective, $OilLvlNormal:obj$ is realised by the oil level controller actuating the control valve mfs:Q5CV2:tra at the outlet of the oil side. The safety of the system is realised by a control valve mfs:V2:bar and a pressure safety valve mfs:Q11PSV:bar which enables gas to flow to a flare if the pressure is too high, but otherwise restricts this flow and thus acts as a barrier.

It is crucial that the model captures certain functionality of the system, such that when the functionality
Figure 3: MFM model of the separation system in the Kairos Workbench editor.
seizes to exist during operation, it can be identified by using the model. The following is a list of such functionality, which should be reviewed, to assess if the model represents these functionalities correctly.

1. The separator pressure Pressure:P2:sto supports the water level control functionality, by enabling outflow of water from the feed side level mfs:h1:tra. A low pressure disables the controller functionality by reducing the outflow through mfs:SDV41036:tra, thus resulting in a high water level.

2. The water level controller enables water and oil separation.

3. The separator wall mfs:WaterOverflow:bar enables oil and water separation, by separating the water on the feed side from the oil on the oil side and vice versa. The functionality of the wall is enabled by maintaining the water level mfs:h1:sto and the oil level mfs:h2:sto. If the water level mfs:h1:sto is too high the water will flow to the oil side and the oil phase will thus contain water.

4. The separator pressure Pressure:P2:sto supports the oil level control functionality by enabling outflow of oil from the oil side level mfs:h2:sto. A low pressure disables the controller functionality by reducing the outflow through mfs:SDV41050:tra, thus resulting in a high oil level.

5. The separator wall supports oil and water separation, by separating the water on the feed side from the oil on the oil side and vice versa. The functionality of the wall is enabled by maintaining the water level mfs:h1:sto and the oil level mfs:h2:sto. If the oil level mfs:h2:sto is too high oil from the oil side will flow to the feed side.

6. The PSV mfs:Q11PSV:bar enables keeping the separator pressure Pressure:P2:sto below a critical level. If the pressure becomes too high, the valve relieves the pressure. If the separator pressure Pressure:P2:sto becomes too high then safety is compromised.

7. The PSV mfs:Q11PSV:bar enables maintaining the separator Pressure Pressure:P2:sto, by acting as a barrier when the pressure is below a critical point. If the valve is breached the pressure Pressure:P2:sto will decrease.

8. The valve mfs:V2:bar enables keeping the separator pressure Pressure:P2:sto below a critical level. If the pressure becomes too high, the valve relieves the pressure. If the separator pressure Pressure:P2:sto becomes too high then safety is compromised.

9. The valve mfs:V2:bar enables maintaining the separator pressure Pressure:P2:sto, by acting as a barrier when the pressure is below a critical point. If the valve is breached the pressure Pressure:P2:sto will decrease.

The MFM model consists of two flow structures, a mass flow structure representing the mixed feed of water, oil and gas, being separated into three different streams, one for water, one for oil and one for gas. The other being an energy flow structure, representing the pressure of the system, governed by the presence
of the mass. However, the pressure enables the flow of mass through the system and is especially a condition for the outflow of liquid from the separator. Wherever balances only have one direct causal relation upstream and one downstream, there is no physical meaning, this is, however, to suppress any inference results from this part, and to adhere to the MFM syntax.

The system features six actuators of which all are valves. All six actuators of the MFM model are tested to produce effect propagations, and in addition, the same valves are tested in K-Spice simulations. The input $X$ for the simulations was sampled for four process conditions: the feed pressure, the feed temperature, the ratio between oil and water (OiW) of the feed, and the actuator step change $\alpha$. A number of $N = 1000$ samples were produced by using LHS for each of the six actuators. This gives 6000 samples to evaluate in total. The feed temperature was varied between 304 and 342 K, the feed pressure between 37 bar and 63 bar, the OiW between 0 and 0.6, and the actuator position between 0 and 100 % open. Thresholds were applied to the simulation output $y_{i,j,k}$. The thresholds were defined as $L_{\text{low}} = -0.01 \%$ and $L_{\text{high}} = 0.01 \%$. The thresholds and the time interval are chosen based on process knowledge and analyses of simulations to investigate the system dynamics. Both thresholds are defined to be close to zero, to only classify near-constant time series as not being causal effects. One reason for having low thresholds is that no process noise is present in simulations. A structured approach has been presented by Yu and Yang [30] for varying method parameters as one-factor-at-a-time to identify a low change rate of the causal metric Transfer Entropy. The values of method parameters are then chosen to minimise the change rate of Transfer Entropy. The thresholds have been chosen to produce a low change rate of the probability. The time interval of the time series $y_{i,j,k}$ was defined by $t_s = 10$ s and $t_e = 50$ s.

5. Results

The result of the causal analysis of the simulations from Nielsen et al. [31] is shown in the QTT in table 5. Each row represents the results for an actuator, for which all simulations classified as a high state for that actuator are represented for each process variable. The first column represents the actuator and a state of the actuator. The remaining columns each represent a process variable and the process variable’s relation to the actuators.

The QTT describes the causal influences which the MFM model should be able to describe, as it represents the most frequent causality exhibited by the system. These states depend on the sampled process conditions, the length of the time series for change detection, and the defined thresholds for classifying the state. The states should be considered in combination with how likely they are to describe the system behaviour.

A probability is determined for the most frequently occurring states for the process variables shown in table 5. The probabilities are shown in table 6. Probabilities exceeding a confidence level of 80 % is
Table 5: Qualitative Trend Table of simulations.

|   | h1 | h2 | P1 | P2 | P3 | Q1 | Q2 | Q3 | Q4 | Q5 | Q6 | Q7 | Q8 | Q9 | Q10 | Q11 |
|---|----|----|----|----|----|----|----|----|----|----|----|----|----|-----|-----|
| HV| +  | +  | +  | +  | 0  | +  | +  | +  | -  | -  | -  | +  | +  | 0   | 0   |
| CV1| -  | -  | -  | -  | 0  | +  | +  | +  | -  | -  | -  | +  | -  | -   | -   | 0   |
| CV2| +  | -  | -  | -  | 0  | +  | +  | +  | -  | -  | -  | +  | -  | -   | -   | 0   |
| V1| -  | -  | -  | -  | 0  | +  | +  | +  | -  | -  | -  | +  | -  | -   | -   | 0   |
| V2| -  | -  | -  | -  | 0  | +  | +  | +  | -  | -  | -  | +  | -  | -   | -   | 0   |
| PSV| -  | -  | -  | -  | 0  | +  | +  | +  | -  | -  | -  | +  | -  | -   | -   | 0   |

marked as yellow. The same accounts for a confidence level of 95% marked by green, indicating that 95% or more of the states were of the same state as the one shown in table 5. Thus 80% and 95% is an indication of a reliable classification of the causal relationship. We assume that the distributions from which the process conditions are sampled are representative of the process operation, with mean values for process conditions representing the normal operation. Thus we assume that the probabilities are shown in table 6 are representative of the most commonly exhibited process behaviour.

A low probability can indicate that it would be advantageous to define regions of the process conditions for which different models should be used, as the causal relationship between cause and effect is non-linear.

Table 6: Probabilities of the analysed causal relations between process variables and actuators. Probabilities equal to or higher than a confidence level of 80% or 95% are indicated by a yellow and green colour.

|   | h1 | h2 | P1 | P2 | P3 | Q1 | Q2 | Q3 | Q4 | Q5 | Q6 | Q7 | Q8 | Q9 | Q10 | Q11 |
|---|----|----|----|----|----|----|----|----|----|----|----|----|----|-----|-----|
| HV| 52 | 53 | 86 | 87 | 87 | 97 | 97 | 52 | 60 | 60 | 51 | 87 | 87 | 87   | 100  |
| CV1| 100 | 98 | 99 | 99 | 100 | 98 | 99 | 100 | 95 | 95 | 100 | 98 | 98 | 98   | 100  |
| CV2| 51 | 94 | 92 | 92 | 100 | 92 | 93 | 53 | 100 | 100 | 96 | 92 | 92 | 92   | 100  |
| V1| 50 | 57 | 96 | 96 | 100 | 96 | 96 | 52 | 78 | 68 | 50 | 99 | 99 | 99   | 100  |
| V2| 73 | 73 | 100 | 100 | 100 | 100 | 100 | 82 | 95 | 84 | 77 | 100 | 99 | 100  | 100  |
| PSV| 95 | 94 | 100 | 100 | 100 | 100 | 100 | 70 | 96 | 98 | 84 | 98 | 99 | 99   | 100  |

5.1. Comparison

The results from testing the MFM model are shown in table 7 in combination with the results from the simulations. The results from the simulations are shown as a single row with a reference to the respective actuator. The rows below represent the results from the MFM model. They are referenced by the actuator name followed by a number that refers to the propagation path number r.
Table 7: Comparison of simulation QTT and MFM QTT.

|   | h1 | h2 | P1 | P2 | P3 | Q1 | Q2 | Q3 | Q4 | Q5 | Q6 | Q7 | Q8 | Q9 | Q10 | Q11 |
|---|----|----|----|----|----|----|----|----|----|----|----|----|----|------|-----|
| HV-1 | + | + | + | + | 0 | + | + | - | - | + | + | + | + | 0 | 0 |
| HV-2 | 0 | + | 0 | 0 | 0 | + | + | 0 | + | + | + | 0 | 0 | 0 | 0 |
| HV-3 | + | 0 | 0 | 0 | 0 | + | + | + | 0 | + | 0 | 0 | 0 | 0 | 0 |
| HV-4 | + | 0 | 0 | 0 | 0 | + | + | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| HV-5 | 0 | + | + | 0 | + | + | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| HV-6 | 0 | 0 | 0 | + | + | + | + | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| HV-7 | 0 | 0 | 0 | + | 0 | + | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| HV-8 | 0 | 0 | 0 | 0 | 0 | + | 0 | 0 | 0 | 0 | + | + | + | 0 | 0 |
| CV1 | - | - | - | - | 0 | + | + | - | - | + | - | - | - | 0 | 0 |
| CV1-1 | - | - | 0 | 0 | 0 | 0 | 0 | + | - | - | - | 0 | 0 | 0 | 0 |
| CV1-2 | - | - | 0 | 0 | 0 | 0 | 0 | 0 | + | 0 | 0 | 0 | 0 | 0 | 0 |
| CV1-3 | - | - | 0 | 0 | 0 | 0 | 0 | + | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| CV1-4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | + | 0 | 0 | + | 0 | 0 | 0 | 0 |
| CV2 | + | - | - | - | 0 | + | + | - | + | + | + | - | - | + | 0 |
| CV2-1 | 0 | - | 0 | 0 | 0 | 0 | 0 | 0 | + | + | 0 | 0 | 0 | 0 | 0 |
| CV2-2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | + | + | 0 | 0 | 0 | 0 | 0 |
| V1 | - | - | - | - | 0 | + | + | - | - | + | + | + | 0 | 0 | 0 |
| V1-1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | + | + | 0 | 0 | 0 |
| V1-2 | 0 | 0 | 0 | - | - | 0 | 0 | 0 | 0 | 0 | + | + | 0 | 0 | 0 |
| V1-3 | 0 | 0 | - | - | 0 | 0 | 0 | 0 | 0 | 0 | + | + | 0 | 0 | 0 |
| V2 | - | - | - | - | 0 | + | + | - | - | + | + | - | - | - | 0 |
| V2-1 | 0 | 0 | - | - | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| V2-2 | 0 | 0 | 0 | 0 | - | 0 | 0 | 0 | 0 | 0 | 0 | 0 | - | 0 | 0 |
| V2-3 | 0 | 0 | - | - | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| V2-4 | 0 | 0 | 0 | - | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | - | 0 | 0 |
| V2-5 | 0 | 0 | 0 | - | - | 0 | 0 | 0 | 0 | 0 | + | + | 0 | 0 | 0 |
| V2-6 | 0 | 0 | - | - | 0 | 0 | 0 | 0 | 0 | 0 | + | 0 | 0 | 0 | 0 |
| V2-7 | 0 | 0 | 0 | - | 0 | 0 | 0 | 0 | 0 | 0 | + | 0 | 0 | 0 | 0 |
| V2-8 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | - | - | 0 | 0 |
| PSV | - | - | - | - | 0 | + | + | - | - | - | - | - | - | 0 | + |
| PSV-1 | 0 | 0 | - | - | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | + |
| PSV-2 | 0 | 0 | 0 | - | - | 0 | 0 | 0 | 0 | 0 | 0 | 0 | - | 0 | 0 |
| PSV-3 | 0 | 0 | 0 | - | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | + |
| PSV-4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | - | - | 0 | 0 | + |
| PSV-5 | 0 | 0 | 0 | - | - | 0 | 0 | 0 | 0 | 0 | 0 | - | 0 | 0 | 0 |
| PSV-6 | 0 | 0 | - | - | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| PSV-7 | 0 | 0 | 0 | - | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| PSV-8 | 0 | 0 | 0 | - | - | 0 | 0 | 0 | 0 | 0 | 0 | - | 0 | 0 | 0 |
| PSV-9 | 0 | 0 | - | - | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
The results from MFM in table 7 for the actuator HV are very similar to those of the simulations, except for the process variables Q4, Q5 and Q6. Table 6 shows that the probabilities for Q4, Q5 and Q6 are low. If more water and oil enters the separator by opening HV, then the water level should increase, and as a result also the oil level. When the water level increases, more water should flow through Q3 and Q6, and when the control reacts by opening CV1, the mass flow through Q3 and Q6 should increase, whereas table 7 shows a decrease. The flow through Q4, Q5, and Q6 should increase as a result of an increased oil level. To reduce the oil level CV2 would open, and Q4, Q5 and Q6 would increase even further. The result should thus be a high state for Q4, Q5 and Q6 independent of the control action. The results from the causal analysis of the simulations are assumed to be incorrect, given that the probabilities of Q4, Q5 and Q6 are low for the actuator HV. Instead, a high state will be assumed for Q4, Q5 and Q6 for the comparison to calculate the model accuracy.

Figure 4: Propagation path CV1-1 from CV1:high to Q6:low.

Propagation path CV1-4 is correct for the actuator CV1 and the process variable Q6, whereas the path CV1-1 is incorrect. If CV1 opens, more water flows through, and Q6 will increase. However for the alternative outcome shown in figure 4, the water level will decrease as more water flows through CV1 (and Q3), and as a result, less water will flow into the oil chamber resulting in a decreased outflow through Q4, Q5 and Q6. This propagation path CV1-1 happens simultaneously with path CV1-4. MFM does however not have any capability of inferring with mediators to determine the state of Q6 based on the conjunctive flows from the oil and the water outlet. However, as the water outlet is considerably larger than the oil outlet, the mass flow of water should determine the state of Q6 rather than the mass flow of oil, given both the oil and the water flow changes. Therefore, the modeller should determine whether this is an unacceptable result or not. Despite being unlikely, as the state of Q6 has a probability of 100 % as shown in table 6, this result is accepted, as an attempt to change it, would influence the propagation path of CV2.

The QTT for CV2 from MFM has no contradictions of the simulation QTT. However many of the process variables show no causal relationship such that CV2 cannot affect them. One issue being that when CV2 opens; the separator pressure P2 decreases, and as a result the mass flow of gas from the separator for Q7,
Q8 and Q9 also decreases. As the mass flow of liquid out of the separator also depends significantly on the pressure P2, the mass flow of water Q3 decreases. All of these effects are not present in the MFM results, whereas they should be. The flow functions mfs:h1:sto and mfs:h2:sto should depend on the separator pressure flow function Pressure:P2:sto, which is a means for maintaining the water and oil levels.

The results of actuator V1 agree well with the validation set. However, the simulation results show either a high or a low state for many of the process variables, whereas missing causal relation in the MFM model results in normal states. As the pressure should decrease in the separator when V1 opens, more water, gas and oil should flow into the separator, thus Q1 and Q2 should increase. However, as the separator pressure P2 decreases, the outflow of Q3, Q4, Q5 and Q6 should decrease. Thus h1 and h2 should be high, and Q3 should be low.

The response of V2 would be expected to be very similar to that of V1, with the difference being, that Q8 and Q9 would decrease, as the mass flow of gas is diverted through Q10, which increases. However, the simulation results show that Q6 increases, which does not seem plausible for similar reasons as argued for V1.

The only contradiction for the PSV is the process variable P3. However, many of the causal relations from the simulation are not present in the MFM model. As the PSV is critical for the plant safety, the flow function mfs:PSV:bar should be prioritised.

P3 seems to be independent of any changes in the system for the simulated process conditions, as the variance of P3 appears to be almost constant during the entire simulation. This behaviour is exhibited both before and after the actuator step change is introduced and is exhibited in all simulations. The MFM model, however, explains that P3 is part of the propagation path for HV, V1, V2 and PSV.

The MFM results from table 7 have been classified as either correct or incorrect by using eqs. (6) to (8). Subsequently, the accuracy has been calculated for every process variable based on the propagation paths for a specific actuator, an average accuracy of each process variable, an average accuracy of each actuator and the accuracy for the entire model by using eqs. (10) to (13). The accuracy of the model, actuators and process variables are shown in table 8.

Based on table 8, Q11 is the process variable with the lowest accuracy followed by Q1, Q2, Q3, P3, h1, Q4, Q5 and then Q6. All these process variables have an accuracy equal to or below 0.5. Thus, these are the primary focus when revising the causal relations. In addition, Q10 and Q11 should be prioritised as they are closely related to the functionality of the safety system.

An obvious way to improve the model would be to introduce a mediate relationship from Pressure:P2:sto
Table 8: Accuracy of MFM model.

<table>
<thead>
<tr>
<th></th>
<th>h1</th>
<th>h2</th>
<th>P1</th>
<th>P2</th>
<th>P3</th>
<th>Q1</th>
<th>Q2</th>
<th>Q3</th>
<th>Q4</th>
<th>Q5</th>
<th>Q6</th>
<th>Q7</th>
<th>Q8</th>
<th>Q9</th>
<th>Q10</th>
<th>Q11</th>
<th>$\bar{A}_q$</th>
</tr>
</thead>
<tbody>
<tr>
<td>HV</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0.94</td>
</tr>
<tr>
<td>CV1</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0.56</td>
</tr>
<tr>
<td>CV2</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0.44</td>
</tr>
<tr>
<td>V1</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0.44</td>
</tr>
<tr>
<td>V2</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0.38</td>
</tr>
<tr>
<td>PSV</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0.44</td>
</tr>
</tbody>
</table>

$\bar{A}_j$ | 0.33 | 0.5 | 0.67 | 0.67 | 0.33 | 0.17 | 0.17 | 0.33 | 0.5 | 0.5 | 0.5 | 0.67 | 0.67 | 0.67 | 0.83 | 0.1 | 0.46 |

This allows propagations to h1, h2, Q3, Q4, Q5 and Q6. This will affect the results of all actuators as they propagate to Pressure:P2:sto. For HV, CV1 and CV2 this would not be a problem, as it produces the same results as the currently existing paths. However for V2 the process variables Q3 and Q6 will contradict the QTT of the simulation. Similarly, Q3 from the MFM propagations will contradict the simulation QTT for the PSV actuator. The following questions thus arise:

- Do we prioritise to have as many similar results between the simulation and MFM as possible (thus avoiding normal states in MFM that contradict high or low states from the simulation)?
- Do we prioritise not having incorrect results?
- Can we somehow simplify the model to not represent the system functionality according to MFM theory to produce the correct results?
- Can we make the model more complex to produce the correct results, by accepting violations of the MFM theory for modelling the physical process as is?
- Can we introduce condition-dependent rules?
- Does MFM lack the capability of representing certain causality or functionality of systems?
- Do we need multiple models, that are tailored for specific conditions or failure modes as suggested by Kirchhiibel et al. [39]?

Therefore, it becomes important to provide something for the modeller, which decisions like this can be based on. The above questions will not be answered here, but it is assumed that various solutions may be beneficial depending on the model application and purpose.

5.2. Model revision

Based on the conclusions from tables 7 and 8, the causal relations of the MFM model shown in fig. 3 are revised. The revised MFM model is shown in fig. C.6 in Appendix C. The actions outlined in section 3.5 are used for the following model revisions:

- The influencer relation between Pressure:bal15:bal $\rightarrow$ Pressure:Q8V1:tra is substituted for a participant relation Pressure:bal15:bal $\rightarrow$ Pressure:Q8V1:tra. This limits propagations to the process variable P3. This means that the pressure in the produced gas outlet cannot be affected by the upstream production.
• A mediate relation is introduced between mfs:h1:sto —□ Pressure:P2:sto. This allows propagations to influence the process variables Q4, Q5 and Q6 from the actuators V1, V2 and PSV. The water level h1 depends on the separator pressure P2 as a low pressure reduces the outflow and thus the water level, and a high pressure increases it.

• The participant relation between mfs:bal12:bal —□ mfs:Q10:tra is substituted for an influencer relation mfs:bal12:bal → mfs:Q10:tra. This allows the actuator V2 to propagate to the process variable Q10. When the flow function mfs:V2:bar is breached, such that gas passes through V2, the flow rate increases for Q10.

• The participant relations between mfs:bal4:bal —□ mfs:LiquidSepIn:tra and mfs:bal2:bal —□ mfs:Q1HV:tra are substituted for the influencer relations: mfs:bal4:bal → mfs:LiquidSepIn:tra and mfs:bal2:bal → mfs:Q1HV:tra. This allows upstream propagations to Q1 and Q2 from the actuators CV1, V1, V2 and PSV. The actuators CV1, V1, V2 and PSV influence the output of gas and water from the system. If these are closed, a limited or no output is produced, whereas if fully open, more gas or water is produced from the system.

The results from the simulations shown in table 5 are compared to those of the revised MFM model according to the same procedure used for the first model version. The resulting accuracy of the revised model is shown in table 9. As can be seen by comparing tables 8 and 9, the accuracy of all actuators has been improved except for that of CV2. Additionally, the accuracy of the process variables h1, h2, P3, Q1, Q2, Q4, Q5, Q6, Q10 and Q11 have been significantly improved. The accuracy of the entire model has improved by 76% from an accuracy of 0.46 to 0.81. However, this is realised by relaxing the proposed condition, that no incorrect results for high or low states are produced for propagation paths. The actuator V2 produces an incorrect propagation path for Q3 and Q6, just as the PSV actuator does for Q3.

Table 9: Accuracy of the revised MFM model.

|   | h1 | h2 | P1 | P2 | P3 | Q1 | Q2 | Q3 | Q4 | Q5 | Q6 | Q7 | Q8 | Q9 | Q10 | Q11 | \( \bar{A}_j \) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| HV | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| CV1 | 1 | 1 | 0 | 0 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 0 | 0 | 0 | 1 | 1 | 0.69 |
| CV2 | 0 | 1 | 0 | 0 | 1 | 0 | 0 | 0 | 1 | 1 | 1 | 0 | 0 | 0 | 1 | 1 | 0.44 |
| V1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 0 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 0.94 |
| V2 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 0 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 0.88 |
| PSV | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 0 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 0.94 |
| \( \bar{A}_j \) | 0.83 | 1 | 0.67 | 0.67 | 1 | 0.83 | 0.83 | 0.33 | 1 | 1 | 0.83 | 0.67 | 0.67 | 0.67 | 1 | 1 | 0.81 |

Any further changes would require, compromising between different actuators. Numerous different approaches to this could be applied. Optimising the mean accuracy of the model or those actuators or process variables related to the greatest risk, or producing multiple models for specific purposes. The aim of this work is to introduce a metric for aiding modellers in revising the model causality, rather than proposing how to compromise between revisions or models.
As a very naive and exhaustive approach, all relations of the model can be changed iteratively to optimise the accuracy metric. However, this would be time-consuming. As previously described, each action can be applied to change the output of the MFM model in a given way. Any relevant actions to achieve a given purpose can thus be applied iteratively to relations on the propagation paths between the actuator and the sensor. In this way, the accuracy metric can be automatically optimised. However, currently, no modelling software for MFM is capable of automating model changes.

6. Conclusion

A probabilistic method for simulating controlled tests of a process system under varying process conditions has been proposed for analysing causal relations. The method was applied to a system for high pressure separation of oil, gas and water to analyse the system causality. By sampling a set of process conditions a high number of tests were simulated in the dynamic process simulator, K-Spice. All process signals were then classified as qualitative and discrete states. The states describe the causal relations of the system between actuators and process variables (sensors).

An MFM model of the system was tested based on a proposed method to produce descriptions from the MFM model similar to those from the simulations. The states from all sampled simulations were converted into the single most probable state and the corresponding probability. A proposed set of rules were used to interpret the MFM propagation paths. The causality derived from the simulations was compared to that of the MFM model. Based on a set of proposed guidelines for revising MFM models, the model accuracy was improved by 76%.

Despite improving the model accuracy, improvements to the method would include a structured approach for revising MFM models. This could involve automating the procedure of applying the proposed revision actions to improve model accuracy. Performing high numbers of simulations is time-consuming and computationally expensive. The subsequent causal analysis is however computationally cheap compared to Transfer Entropy; the most widely applied method for process systems. With efficient test designs, the proposed method will require much less computational time compared to Transfer Entropy when the system size scales. The process conditions are crucial to the validation and application of the MFM model. Therefore, further effort should focus on defining the process condition range of MFM models. The concept of producing multiple models to represent operational modes [39] could be extended to validate MFM models on subsets of process conditions. The method presented here can thus be validated on a subset of the sampled process conditions.

Both the simple and complex example showed that this method can be applied to successfully validate and improve the causality of MFM models based on a stochastic approach to carry out controlled experiments in simulations.
7. Acknowledgements

This work was supported by the Danish Hydrocarbon Research and Technology Centre and Otto Mønsteds Fond.

References


## Appendix A. Flow function to component associations

<table>
<thead>
<tr>
<th>Flow function</th>
<th>Name</th>
<th>Component</th>
</tr>
</thead>
<tbody>
<tr>
<td>mfs:h1:sto</td>
<td>h1</td>
<td>Water level sensor</td>
</tr>
<tr>
<td>mfs:h2:sto</td>
<td>h2</td>
<td>Oil level sensor</td>
</tr>
<tr>
<td>mfs:Q1HV:tra</td>
<td>Q1</td>
<td>Flow rate sensor</td>
</tr>
<tr>
<td>mfs:Q2:tra</td>
<td>Q2</td>
<td>Flow rate sensor</td>
</tr>
<tr>
<td>mfs:Q3CV1:tra</td>
<td>Q3</td>
<td>Flow rate sensor</td>
</tr>
<tr>
<td>mfs:Q4:tra</td>
<td>Q4</td>
<td>Flow rate sensor</td>
</tr>
<tr>
<td>mfs:Q5CV2:tra</td>
<td>Q5</td>
<td>Flow rate sensor</td>
</tr>
<tr>
<td>mfs:Q6:tra</td>
<td>Q6</td>
<td>Flow rate sensor</td>
</tr>
<tr>
<td>mfs:Q7:tra</td>
<td>Q7</td>
<td>Flow rate sensor</td>
</tr>
<tr>
<td>mfs:Q8V1:tra</td>
<td>Q8</td>
<td>Flow rate sensor</td>
</tr>
<tr>
<td>mfs:Q9:tra</td>
<td>Q9</td>
<td>Flow rate sensor</td>
</tr>
<tr>
<td>mfs:Q10:tra</td>
<td>Q10</td>
<td>Flow rate sensor</td>
</tr>
<tr>
<td>mfs:Q11PSV:tra</td>
<td>Q11</td>
<td>Flow rate sensor</td>
</tr>
<tr>
<td>Pressure:P1:sto</td>
<td>P1</td>
<td>Pressure sensor</td>
</tr>
<tr>
<td>Pressure:P2:sto</td>
<td>P2</td>
<td>Pressure sensor</td>
</tr>
<tr>
<td>Pressure:P3:sto</td>
<td>P3</td>
<td>Pressure sensor</td>
</tr>
<tr>
<td>mfs:Q1HV:sto</td>
<td>HV</td>
<td>Startup hand valve</td>
</tr>
<tr>
<td>mfs:Q3CV1:tra</td>
<td>CV1</td>
<td>Water level control valve</td>
</tr>
<tr>
<td>mfs:Q5CV2:tra</td>
<td>CV2</td>
<td>Oil level control valve</td>
</tr>
<tr>
<td>mfs:Q8V1:tra</td>
<td>V1</td>
<td>Startup pressure control valve</td>
</tr>
<tr>
<td>mfs:V2:bar</td>
<td>V2</td>
<td>Flare pressure safety control valve</td>
</tr>
<tr>
<td>mfs:Q11PSV:bar</td>
<td>PSV</td>
<td>Flare pressure safety valve</td>
</tr>
</tbody>
</table>
Appendix B. P&ID of case study system

Figure B.5: P&ID of case study system.

Appendix C. Revised MFM model
Figure C.6: Revised MFM model.