

# SDG and qualitative trend based model multiple scale validation

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**Abstract.** Verification, Validation and Accreditation (VV&A) is key technology of simulation and modelling. For the traditional model validation methods, the completeness is weak; it is carried out in one scale; it depends on human experience. The SDG (Signed Directed Graph) and qualitative trend based multiple scale validation is proposed. First the SDG model is built and qualitative trends are added to the model. And then complete testing scenarios are produced by positive inference. The multiple scale validation is carried out by comparing the testing scenarios with outputs of simulation model in different scales. Finally, the effectiveness is proved by carrying out validation for a reactor model.

## 1 Introduction

With the continuous development of science and technology, simulation technology has made great progress, and plays an increasingly important role in the economy, military, transportation, chemical and other industries. Since the emergence of simulation technology, how to ensure the validity and accuracy of the simulation model is a very important issue. The evaluation of the effectiveness of the simulation model mainly includes three parts: verification, validation and accreditation<sup>[1]</sup>. Verification is to verify whether the conversion from the mathematical model to the computerized model has a certain degree of accuracy. Validation refers to whether the model is a true description of the original system and expresses the real world<sup>[2]</sup>. Accreditation is made by experts of the domain to evaluate the simulation model to determine whether the simulation model has met the requirements. The specific relationship is shown in Figure 1.

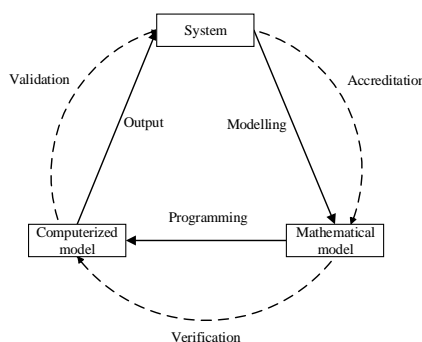


Figure:1 The relationship of Simulation modeling and verification, validation and accreditation

Verification and validation are more dependent on the method than the model accreditation of expert experience. Among them, the model verification is mainly the model software verification. All the verification methods in the software engineering can be used to examine the model, including: programmer self- verification, consistency test, top-down test, symbol analysis and so on<sup>[3][4]</sup>. The method of model verification mainly includes subjective verification method and mathematical statistics-based method<sup>[5][6]</sup>. Subjective verification methods include: subjective validity evaluation, theoretical comparison method, algorithm by hand, model comparison and so on. The main drawback of subjective verification method is that it relies heavily on the experience of the examiner, and the effectiveness of the model validation depends largely on the level and experience of the validator. The method based on mathematical statistics mainly depends on the quantitative analysis of various mathematical tools. At the same time, with the emergence of new simulation technology, such as Agent-based simulation, it has put forward a higher demand to the verification model<sup>[7][8]</sup>.

In fact, from the essence of the validation model, the purpose of validation is to verify that the model can accurately represent the actual system in the context of modeling purposes. However, there are deficiencies in the current validation method:

(1) Validation needs to be compared with the real system, relying heavily on real measurement data. However, the actual real data is not easy to obtain. In terms of chemical equipment or production processes, steady-state production data is also relatively easy to obtain, but the data under a variety of different conditions (especially the failure, abnormal data after the occurrence) is difficult to obtain, so that it has negative effect on the model validation.

(2) Even if the real data has been gotten, how to ensure the integrity of the validation data is a problem. That is, how to ensure that the data used to validate the simulation model contains all the real system of the operation. This is a big challenge to the current model validation method.

(3) The current validation method at different scales is scare, namely, the definition of “similarity degree” is used to define and describe the similarity of different levels.

(4) The current validation method, especially subjective emanation, which is highly dependent on the experience of the person. The validation results of different person may be inconsistent, affecting the effect of validation model.

Aiming to solve the above problems, this paper proposes a SDG and qualitative trend based model multiple scale validation. Firstly, the SDG model with qualitative trend is established for the real system. The model is a qualitative description of the real system and incorporates some quantitative information. The changes of different nodes in the model and positive inference can produce complete testing scenarios. Then the scenarios with the change trend are compared with the simulation data of the simulation model, and the model is verified by comparing the similarity degree from different scales. Finally, a reactor model is proved that the method has the advantages of completeness, multi-scale and little dependence on experience.

The main structure of the thesis is as follows: The first part is introduction. The second part introduces the SDG and qualitative trend based validation model. On the basis of validation model, the third part introduces the multiple scale validation method based on this model. The fourth part adopts a reactor to validate; the last part is the conclusion.

## **2 SDG and qualitative trend based validation model**

### *2.1 The basic concept of SDG*

The SDG model is a qualitative causal model that describes the influence of the system. The model can be used for positive and negative inference. The SDG model uses nodes to represent variables in the system. Node states are represented by "+", "-", "0", and the relationship between nodes is expressed by "+" and "-". The model can describe the current state of the system through the relationship between the nodes (called branches). And through the positive inference can be determined under different circumstances, the system different state.

With the advantages of modelling convenience and the completeness of system state, SDG model is widely used in simulation modelling, fault diagnosis and safety analysis. However, due to the traditional SDG model, the description of node state and node relation is too simple. While the modelling simplicity is ensured, a lot of information is lost, which makes the model not accurate enough. Therefore, some scholars have begun to study some quantitative information added to the SDG model<sup>[9][10]</sup>, to further improve the model of the variable relationship, the state of the system to make it more accurate.

## 2.2 SDG and qualitative trend based validation model

Model validation is to validate whether the simulation system can accurately represent the actual system, because the real system data, especially in various states of the data is difficult to obtain, therefore, a model to replace the real system for validation is proposed. The model needs to have the following characteristics: (1) Be able to Describe the states of the real system completely; (2) The modeling is simple and dependent little on people's experience. The SDG model with qualitative trend has the above characteristics, so the SDG model is adopted as the validation model.

On the basis of the traditional SDG model, the qualitative trend is used instead of "+", "-" and "0" to describe the state of the node. While the use of qualitative trends instead of "+", "-" to describe the relationship between nodes. Qualitative trends are described by the following 6 basic trend elements and their combinations, as shown in Figure 2.

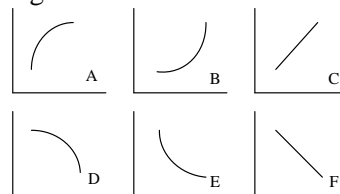


Figure 2: 6 basic trend elements

Using the six basic trend elements in Figure 2 to describe the state of every node in the SDG model and the relationship between nodes, in some complex cases, the combination of six primitives can be used to express the state of the node in detail. Compared with the traditional state, the qualitative trend can describe the node state and the relationship between the nodes in detail and the description of the system state is more accurate.

SDG validation model specific modeling method is shown in Figure 3.

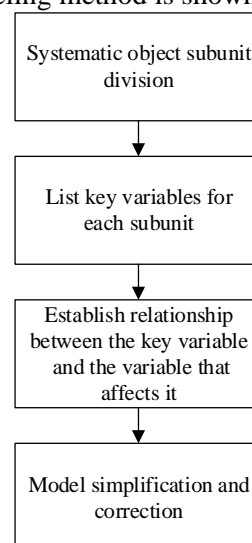


Figure 3: SDG modelling method

Among them, after the establishment of the model, we need to simplify the model several times to ensure that the model can meet the requirements.

### 3 SDG and qualitative trend based model multiple scale validation

SDG and qualitative trend based model multiple scale validation is divided into three steps: Firstly, the SDG model of the system is established. Then, the traditional rules and the qualitative trend based positive inference are carried out on the SDG model, and the complete scenarios (qualitative trends of all nodes in various states) are obtained. Finally, the trends of the generated model are compared with the qualitative trends extracted in the simulation model, and the availability of the simulation model is validated.

#### 3.1 Qualitative trend based positive inference

In order to obtain complete scenarios for model validation, qualitative trend based positive inference on SDG model is needed. The main algorithm flow is as follows.

##### (1) The acquisition of the primary validation scenarios

Traverse the SDG model, set every node to “+” or “-”, and according to the traditional compatibility rules (The state of the downstream node = the status of the upstream node \* the sign of the branch), positive inference is used to obtain the status of each node under the deviation (“+” or “-”). So as to get the scenarios under each bias. This step is based on the traditional compatibility rules, in order to obtain the scenarios for the initial level of model validation. The primary scenarios are used to compare the scenarios once the trend scenarios cannot meet the requirements.

##### (2) The acquisition of the qualitative trend based validation scenarios

A. Traverse the SDG model, for each node, set to one of the six trend elements, and carry out a positive inference. According to the positive inference rules generated by the impact of the node trend. This node acts as the current node and continues positive inference until the consequences node is reached. That is, no node is affected by the node. All passed nodes are marked as searched.

B. Return from the current node to its upstream node and continue inferring until all nodes are marked as searched.

C. Set the other trend base for the current node and continue the inference, until the six elements of the deviation are inferred.

D. Continue to set the trend of other nodes and infer, until all the nodes have been processed.

E. Each trend deviation corresponds to a scenario, then they are stored for model validation.

The qualitative trends based inference rules need to be divided into two cases:

1) There is an influence on the relationship between the upstream and the downstream node. There is an only one branch pointing to the downstream node. The trend of the downstream node is shown in Table 1.

Table 1: Qualitative trends based inference rules

Branch trend \ Node state	A	B	C	D	E	F
A	A	C	A	F	E	E
B	C	B	B	D	F	D
C	A	B	C	D	E	F
D	F	D	D	B	C	B
E	E	F	E	C	A	A
F	E	D	F	B	A	C

2) The branch that affects the downstream node is more than one.

When the downstream node is affected by more than one branch, the trend state of the node is determined by the state of all upstream nodes and the trend of the branch. As shown in Equation 1:

$$S_{effect} = \sum_{i=1}^N S_{causei} \quad (1)$$

Where  $S_{effect}$  is the downstream node state and  $S_{causei}$  is the state of the downstream node under the

single action of the  $i$ th upstream node. Suppose there are a total of  $N$  upstream nodes. The state of the downstream node under the action of a single upstream node is determined by Table 1. The state rules of the superposition of multiple upstream nodes are shown in Table 2.

Table 2: Trend status overlay rules

Node trend \ Node trend	A	B	C	D	E	F	?
A	A	C	A	?	?	?	?
B	C	B	B	?	?	?	?
C	A	B	C	?	?	?	?
D	?	?	?	D	F	D	?
E	?	?	?	F	E	E	?
F	?	?	?	D	E	F	?
?	?	?	?	?	?	?	?

A status of "?" indicates that the state of the node cannot be determined. When the upstream node state is "?", its downstream node status is also "?". Table 2 contains the rules for the superimposition of two upstream node states on the same downstream node state, and this rule is also used to multiple nodes. Through the positive inference, you can get a variety of conditions under the complete scenarios.

### 3.2 Qualitative trend extraction algorithm

In order to compare with the qualitative trend in the simulation model, qualitative trend extraction algorithm is needed to extract the qualitative trend of the simulation model data. The qualitative trend is obtained by using the extraction algorithm of qualitative trend analysis with sliding window<sup>[11]</sup>.

### 3.3 Method of model multiple scale validation

After obtaining the complete scenarios by positive inference and extracting the qualitative trends in the simulation model, you can compare the trend to determine whether the simulation model can accurately simulate the real system. In order to describe the degree of similarity at different scales, the degree of similarity is defined as 3 levels. The specific definition is as follows.

Level 1 similarity: The symbols for the current node are the same (Greater than the upper limit is "+", less than the lower limit is "-", between the upper and lower limits is "0"). Level 1 similarity is the current moment, which is the consistency between the state of the variables in the scenario and the state of the variable in the simulation, is the original level similar.

Level 2 similarity: The first derivative of the two trends is the same, that is, the direction of the change is consistent. Such as A, B, C are all rising changes. D, E, F the same reason. Examine the degree of change in the direction of change over a period of time.

Level 3 similarity: The first and second derivatives of the two trends are the same. Such as A and A, B and B. And then examine the degree of similarity in a change over a period of time.

When comparing, first determine whether the trend can meet the level 2 similar, if satisfied, then determine whether to meet the level 3, if cannot meet the level 2, then determine whether to meet the level 1.

In order to quantify the degree of similarity, a weight is assigned to each level, that is, the level 1 similarity is 1, Level 2 similarity is 2, Level 3 similarity is 3 and the dissimilarity is 0. For each scenario, suppose there are  $N$  variables, then the similarity degree between the scenarios and simulation system qualitative trend is defined as:

$$S_{\text{scenario}} = \frac{1}{N} \sum_{i=1}^N S_i \quad (2)$$

$S_{\text{scenario}}$  is a similar weight of the simulation system and the real system for a scenario.  $S_i$  is the similar weight of the  $i$ th simulation system variable to the real system variable. Suppose there are  $M$  scenarios, then the simulation system and the real system similar weight:

$$S_{total} = \frac{1}{M} \sum_{j=1}^M \left( \frac{1}{N} \sum_{i=1}^N S_i \right)_j \quad (3)$$

Depending on the different values of  $S_{total}$ , different similarity levels are determined. As shown in Table 3.

Table 3: Similarity level definition

Ranges	Similarity level
$S_{total} < 0.5$	0 (not similar)
$0.5 \leq S_{total} \leq 1.5$	Level 1
$1.5 < S_{total} \leq 2.0$	Level 2
$S_{total} > 2.0$	Level 3

The simulation system to the real system description reached a high degree when the trend comparison reaches the level 3 similarity. At the same time, the range of the value of each level in Table 3 can also be changed flexibly according to the specific circumstances. When the requirements is simple, such as just requiring, the simulation system for the principle of validation and demonstrates some simple cases, you can reduce the scope of the value. For the simulation system with more stringent requirements of the situation, you need to improve the scope requirements.

In summary, SDG and qualitative trend based model multiple scale validation method shown in Figure 4.

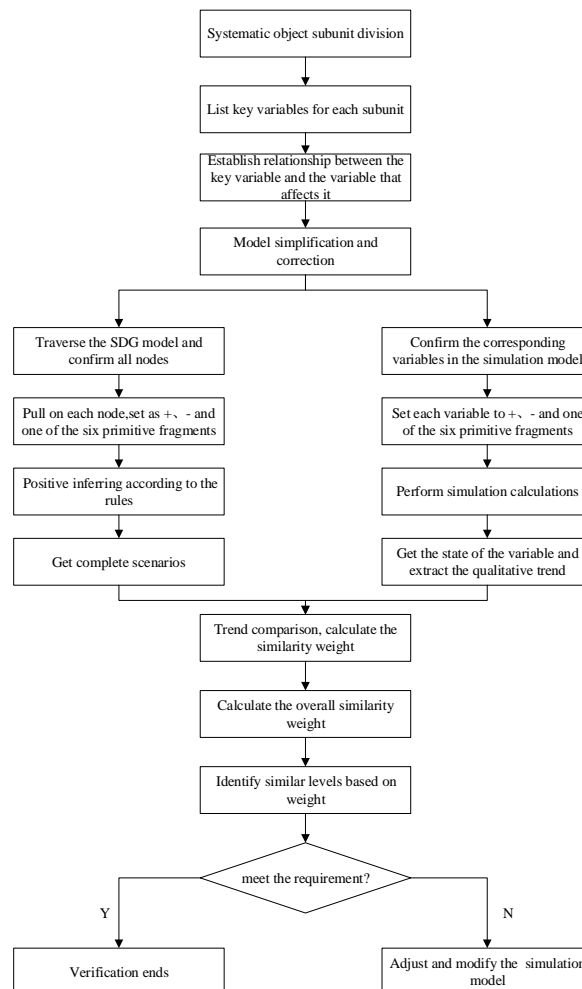


Figure 4: SDG and qualitative trend based model multiple scale validation flow

#### 4 Case study

The above method is applied to the validation of a reactor simulation model. This model is one of the subunits in the SMPT1000 (Advanced Multifunction Process Control Training System). The system flow is shown in Figure 5.

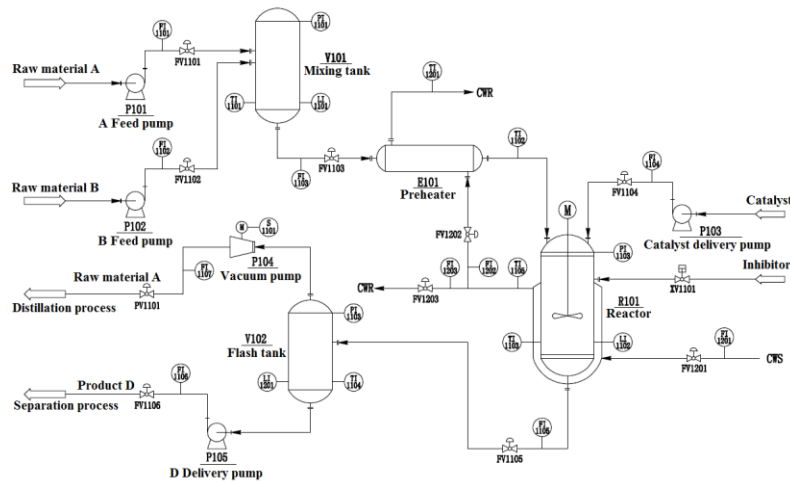


Figure 5: Reactor flow chart

As shown in Figure 5, the system simulates the process of forming D and E under the action of the catalyst C by the materials A and B. A, B is put into the buffer tank, and then into the reactor, under the action of the catalyst reaction. The product mixture enters the flash tank for flashing, where material A is used for the recovery of raw materials from the top, the main product D from the bottom of the tank into the next refining process. The list of variables is shown in Table 4.

Table 4: List of main variables for the reactor system

Variable Tag	Description	Variable Tag	Description
FI1106	Mixed product flow	LI1102	Reactor level
FI1101	Raw material A flow	LI1201	Flash tank level
FI1102	Raw material B flow	TI1101	Mixing tank temperature
FI1103	Raw material mixed feed flow	TI1102	Feed the preheater temperature
FI1104	Catalyst C flow rate	TI1103	Reactor temperature
FI1105	The bottom of the reactor generates the liquid flow	TI1104	Flash tank temperature
FI1107	Flash tank top circulation raw material flow	TI1105	Closed cycle return water temperature
FI1201	Jackets circulating water flow	TI1201	Loop back to the preheater temperature
FI1202	Cycle back to the preheater flow	PI1101	Mixing tank pressure
FI1203	Loop backwater to sector traffic	PI1102	Reactor pressure
LI1101	Mixing tank level	PI1103	Flash tank pressure

First the SDG model of the simulation object is established. As shown in Figure 6.



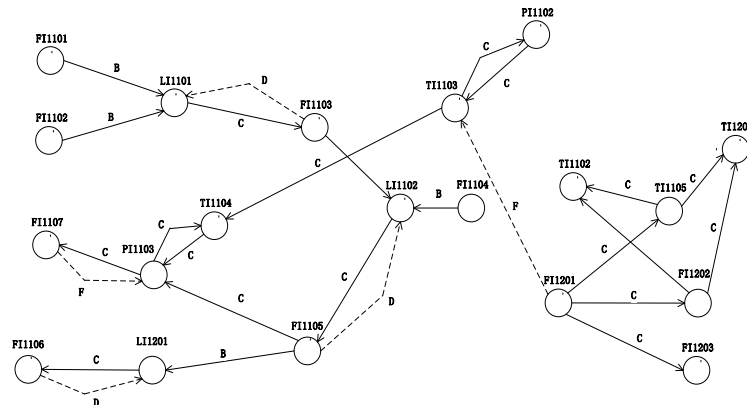


Figure 6: SDG model

Firstly, we need to set the deviation of "+" and "-" for each node, then 40 primary validation scenarios will be obtained by positive inference on the basis of the SDG model. Then we set one of the six trend elements for each node, 120 trend scenarios obtained by positive inference. Simulate these scenarios in the simulation model, extract the qualitative trend, and compare with the scenarios generated by the SDG model to calculate the similarity weights. Taking the "+", "-" and 6 kinds of trend elements for the inferring of the cooling water feed flow FI1201 as an example, the 8 scenarios are shown in Table 5. Only the affected variables are listed.

Table 5: scenarios through positive inference

N O	FI 12 01	FI 12 03	FI 12 02	TI 11 05	TI 12 01	TI 11 02	TI 11 03	PI 11 02	TI 11 04	PI 11 03	FI 11 07
1	+	+	+	+	+	+	-	-	-	-	-
2	-	-	-	-	-	-	+	+	+	+	+
3	A	A	A	A	A	A	E	E	?	?	?
4	B	B	B	B	B	B	D	D	?	?	?
5	C	C	C	C	C	C	F	F	?	?	?
6	D	D	D	D	D	D	B	B	?	?	?
7	E	E	E	E	E	E	A	A	?	?	?
8	F	F	F	F	F	F	C	C	?	?	?

The "?" state in the table indicates that the trend of the node cannot be determined under the influence of multiple nodes. For FI1201, the trend of each of the variables in the scenario 3-8 is compared with the trend of the variables in the simulation system and the weights are calculated. For variables that do not meet the level 2 similarity, using the state of the variables in the scenario 1-2 to determine whether to meet the level 1 similarity and calculate the weights. For the 6 basic trend changes of FI1201, the similarity weight is about 2.18. In the same way, after calculating other variables to produce 6 kinds of trend elements, the similarity weights of the variables of the simulation system are calculated. Finally, the similarity level between the simulation system and the real system is 3.

## 5 Conclusion

A SDG and qualitative trend based model multiple scale validation is proposed for the lack of completeness of the traditional model validation method, lack of multiple scale validation method and over-reliance on human experience. This method is divided into three steps: Firstly, the SDG model of the real system is established and the qualitative trends are added to enrich the expression of the model. The second step is to generate the complete scenarios with the trends through the change of the node and the positive inference. The third step will be the scenarios and simulation system trends for



multiple scale comparison to validate the accuracy of the simulation model. The results show that the proposed method can produce a complete and multiple scale test and validation of the simulation model, and it can be applied to the validation of the simulation model.

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