



NATIONAL TRANSPORTATION SAFETY BOARD

**Investigative Hearing**

Norfolk Southern Railway general merchandise freight train 32N  
derailment with subsequent hazardous material release and fires,  
in East Palestine, Ohio, on February 3, 2023

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Title

**Predicting Runaway Reaction in PVC**

# Predicting Runaway Reaction in PVC Batch Process using Support Vector Machine

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**Abstract-** In this paper, predicting runaway reaction in a PVC batch process using Support Vector Machine is reviewed. The use of support vector machines (SVM) is considered for their simpler design and implementation, and for allowing the better handling of complex and large data sets. In order to compare results with previously reported works, a case study such as the PVC batch process is considered. SVM achieves consistent and promising results.

**Keywords-** runaway reaction; support vector machine (SVM); batch process

## I. INTRODUCTION

Batch chemical industries have been attracting for safety engineers since they pose a number problem in behavior and operation. Compare to the continuous plants, a batch process has unique characteristics, behavior of process changes dynamically, role of operators, and the change of process variable [1]. Besides using the hazardous material, a batch abnormality can be caused by the deviation of process variable and plant mal-operation [2]. A process variable deviation occurs during batch process and it becomes a significant factor for the safety issues in the plants. The deviations tend to influence plant operation and change the situation into abnormal state and contribute in damaging the plants.

Towards fulfill the global requirement, the companies should ensure safety and quality for their plant. Over the years, product quality has become primary focus due to it gives direct impact to benefit. However, due to aging and reducing of plant reliability, safety problems will emerge in some existing batch plants. In this paper, a novel method in batch plant hazard identification is proposed using advance technique in risk assessment. Some conventional methods such as Failure Tree Analysis, Event Tree Analysis, and Human Reliability Analysis are still used in industries. However, these method are capable only both in pre-accident and post-accident situation [3], and do not consider the real condition of the plants, it is difficult to analyze accurately the real time process and integrate the results with the prior condition of the processes. For example, Event Tree Analysis, it is usually implemented in two stages, pre-incident and post-incident analysis. Pre-incident is intended to identify hazards that vulnerable to the plant system, environment, human, etc., the results should be considered as the input

for operational stage. The post-incident analysis is intended to evaluate the probability of occurrence, the results of this analysis should be considered as historical data that guides the operational stages for the near future. On the other hand, identification of hazards based on the operational stage condition is essential to avoid the consequences and revise the recent condition for safety improvement program. As solution of this problem, a fault propagation assessment technique can be used in analyzing accurately the abnormalities. Fault propagation manipulates information from sensor and batch recipe system to estimate the performance of safety objects in handling abnormality [4]. The aim of real time hazard identification is to predict the condition patterns prior to accident occurs, these patterns are expressed in indices and obviously, the optimal policy for plant safety design and maintenance can be decided in avoiding the hazardous outcomes. The real-time applications of performance reliability prediction are useful in operation control as well as predictive maintenance [5].

One of the potential accidents in the batch plants is runaway reaction. Runaway reaction has been reported as potential hazard in the batch process. Based on the newest data, runaway reaction leads to fires and explosion, where the majority of incidents occurred during normal operation and two main causes were investigated as runaway reaction and overflow of material. As case study, runaway incidents in PVC batch process are investigated at VCM charging line that potential contributes to overflow of monomer and lead to runaway reaction.

The objective of this study is to evaluate the application of Support Vector Machine (SVM) for predicting runaway reaction in a PVC reactor. This research is a continuation of our research before [6]. SVM models, which are based on the statistical learning theory, are a new class of models that can be used for predicting the values.

## II. METHODOLOGIES

### A. Literature Review

In the area of hazard identification, there are two main tasks, (i) identification of specific undesirable consequences and (ii) identification of material, system, process and plant characteristics that could produce those

consequences. A hazard identification tool performs the possible deviations from normal operation are listed and the possible abnormal causes and the adverse consequences for these deviations are identified. The most popular methodology for hazard identification is hazard and operability studies or HAZOP.

Event propagation or accident progression can be determined as the failure of safety systems in preventing or mitigating the hazards. Therefore, the concept of fault propagation is relevant to this situation and can be adopted as a model and tool in hazard identification. Kelly and Lees introduced the term of fault propagation and it was a model that use of functional equations that describe how an output variable is affected by the input variables. A functional equation describes the relation between an output variable of a unit and the input and other output variables of the unit. A propagation equation may be converted directly into mini FTA [7].

SVMs are a set of related supervised learning methods used for classification and regression, and possess the well-known ability of being universal approximators of any multivariate function to any desired degree of accuracy. It has been found that SVMs show better or comparable results than the outcomes estimated by neural networks and other statistical models.

SVM are based on the structural risk minimization principle from the statistic learning theory and, in their basic form, they learn a linear hyperplane that separates a set of positive examples from a set of negative examples with maximum margin (the margin is defined by the distance of the hyperplane to the nearest of the positive and negative examples). This learning bias has proved to have good properties in terms of generalization bounds for the induced classifiers. The linear classifier is defined by two elements: a weight vector  $w$  (with one component for each feature), and a bias  $b$  which stands for the distance of the hyperplane to the origin. The classification rule assigns +1, to a new example  $x$ , when  $f(x) = (x,w) + b \geq 0$ , and -1 otherwise. The positive and negative examples closest to the  $(w,b)$  hyperplane are called support vectors [8].

## B. Proposed Methodology

In this paper, a model of support vector machine (SVM) that can be used for prediction runaway reaction in a polyvinyl chloride reactor had developed. The use of SVM model is considered for their simpler design and implementation, allowing the better handling of complex and large data set, and for comparing with Back-Propagation Neural Network models documented in previous research. A case study is focused on the runaway incident at polyvinyl chloride (PVC) batch process which is consumed the hazardous material, vinyl chloride monomer (VCM).

## III. MODEL IMPLEMENTATION WITH CASE STUDY-PVC BATCH PLANT

In this paper, I study on predicting runaway reaction in PVC batch process using Support Vector Machine. Case study is simplifying batch reactor of PVC plant as has shown in Figure 1. The temperature data (normal and runaway) are used to illustrate the performance of the proposed model. This study describes a classification methodology based on SVM, which using SVM classifier with linear kernel function and one-norm function.

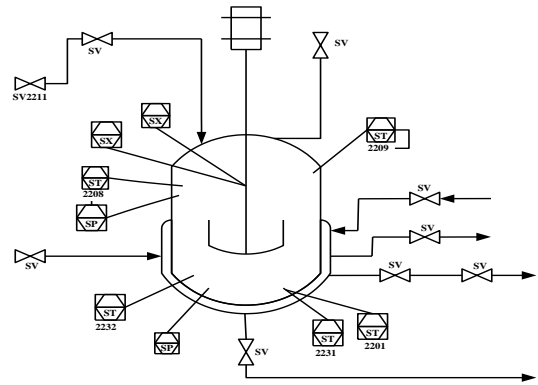


Figure 1 Batch reactor of PVC plant diagram

Steps for classify data using support vector machine are [9]:

- Load the data (temperature of vessel)
- Create *data*, a two-column matrix containing sepal length and sepal width measurements
- From the *species* vector, create a new column vector, groups, to classify data into two groups: Normal and Abnormal
- Randomly select training and test sets
- Use the *svmtrain* function to train an SVM classifier using a linear kernel function and plot the grouped data.

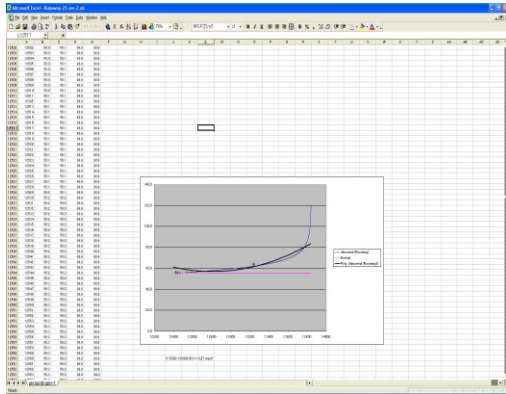


Figure 2 Data's temperature in reactor PVC batch plant

In this implementation, I have used data's temperature in reactor PVC batch plant as shown in Figure 2. The data's temperatures consist of normal and runaway condition. Figure 3 represent the simulation result of train an SVM classifier using a linear kernel function from temperature data in reactor PVC batch plant.

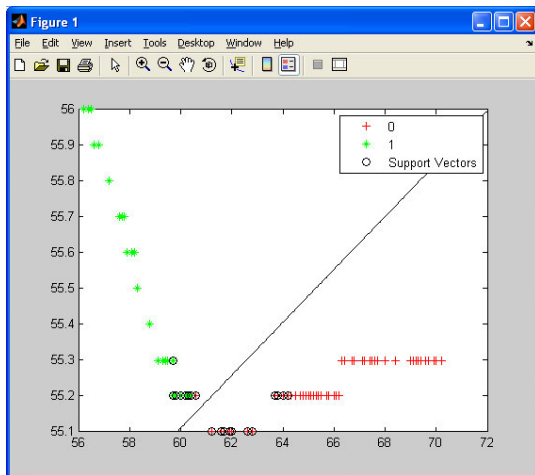


Figure 3 Simulation result of train an SVM classifier using a linear kernel function from temperature data in reactor PVC batch plant

Figure 4 represent the simulation result of SVM classify the test set using a support vector machine from temperature data in reactor PVC batch plant. From this figure have been found an optimal separating hyperplane by maximizing the margin between the separating hyperplane and the data. In this case, the y- axis is for normal temperature and the x-axis is for the runaway temperature (in degree Celsius).

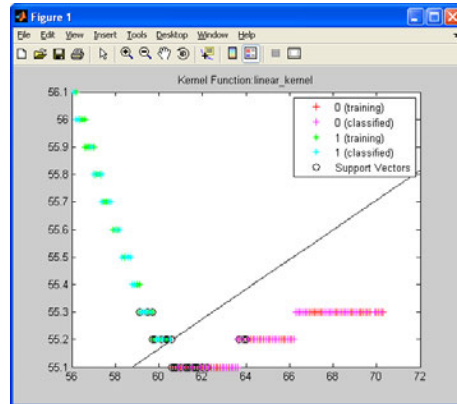


Figure 4 Simulation result of SVM classify the test set using a support vector machine from temperature data in reactor PVC batch plant

After that, we can also make an evaluation the performance of the classifier with formula and result (Matlab execution):

```
>> classperf(cp,classes,test);
>> cp.CorrectRate
```

ans =  
0.9867

Figure 5 and Figure 6 represent the simulation result of hard margin SVM classifier by using a one-norm. For evaluating the performance of the classifier, we use the formula and result (Matlab execution):

```
>> classperf(cp,classes,test);
>> cp.CorrectRate
```

ans =  
0.9867

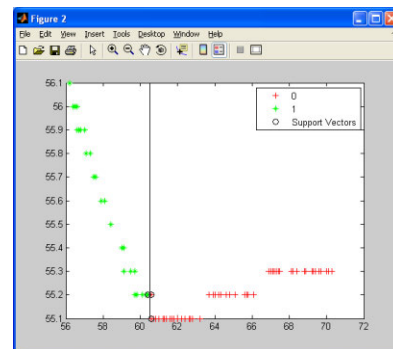


Figure 5 Simulation result of SVM hard margin SVM classifier (svmtrain) by a using one-norm

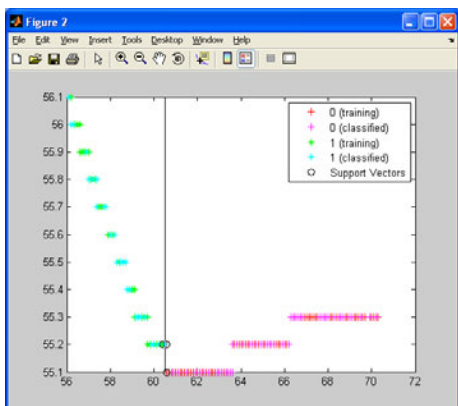


Figure 6 Simulation result of SVM hard margin SVM classifier (svmclassify) by using a one-norm

From simulation result of SVM classify the test set using a support vector machine from temperature data in reactor PVC batch plant, we have got that the optimal hyperplane is  $F(x) = 60.6$  °C. From the data, we note that the temperature  $60.6$  °C occurred when the time process is 13105 s. If we assume that runaway reaction will start when the temperature threshold value is  $70$  °C (13614 s), then we have time for anticipating the runaway reaction is about 8.5 minutes.

#### IV. DISCUSSION

In this paper, a new approach for predicting runaway reaction has been proposed based on linear kernel function SVM classifier and one-norm function SVM classifier. From these methods we can compare that both results are same good as shown by evaluation the performance of the classifier with formula i.e., 0.9867. If we compare the simulation result of SVM classifier using linear kernel and SVM classifier using one-norm (between Fig. 4 and Fig. 6), then we mention that SVM classifier using one-norm is better for calculating of anticipating runaway reaction.

We also mention that the use of SVM is simpler design and implementation. We can develop early warning detection system base on calculation of time for anticipating the runaway reaction. Therefore, SVM method effectively can help and support the decision-making of plant operators.

#### V. CONCLUSIONS

We have presented the study on predicting runaway reaction using Support Vector Machine. The use of support vector machines (SVM) is considered for their simpler design and implementation, and for allowing the better handling of complex and large data sets. From the simulation result of SVM classify the test set using a support vector machine from temperature data in reactor PVC batch plant, we found that the prediction of runaway reaction can be detected earlier and safer i.e., we have time for anticipating the runaway reaction is about 8.5 minutes.

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