



## PREDICTIVE ANALYTICS IN STABILITY STUDIES

Pharmaceutical or consumer product shelf-life for any new variant is subject to its Active Pharmaceutical Ingredients (API) and various environmental/storage conditions like temperature, humidity and packaging material. Any of these factors can change the chemical stability of a drug or a consumer product. As a result, long-term testing and accelerated testing need to be conducted to determine the shelf life of the new product or a new variant. This POV presents factors that can affect a product and shows how Machine Learning (ML) can be adapted to predict changes to the API. Thus, any change to the new product or variant can be studied with the help of ML analytics and can act as a tool based on the historical LIMS database. Stability analytics aims to build a ML model which can predict the stability value of the components and how they react in contrast conditions.

# What is Predictive Modeling

Predictive modeling is a branch of advanced analytics that predicts future behavior and events. Predictive analytics uses many techniques from data mining, statistics, modeling, ML and artificial intelligence (AI) by analyzing historical and current data and generating a model to predict future outcomes. Simply put, predictive analytics uses past trends and applies them to the future. The patterns found in historical data can be used to identify risks and opportunities for the future. By successfully applying predictive analytics, the business can effectively interpret past stored data for its benefit. Predictive modeling helps the organization become proactive, forward-looking, and anticipate outcomes and behaviors based on data and not on assumptions. It goes further and helps the organization to take beneficial actions.

## How it works

In the as-is scenario, traditional testing, including accelerated testing, is made to run on all components to determine the shelf life of a product. This approach makes the as-is scenario very time consuming. On the other hand, in to-be scenario, we have an ML model that predicts the stability value using data fed. We can determine which components have passed or failed, mandating traditional testing only on failed components. In figure 1, the model predicts that 98% of the components have passed, i.e., the stability value predicted for these components lies between the upper and lower limits. So, traditional testing must be performed only on the remaining 2% of the failed components. This reduces effort by 98%\*.

\*Note: Results may vary depending on the product data and its components

Figure 1 Predictive modeling at work

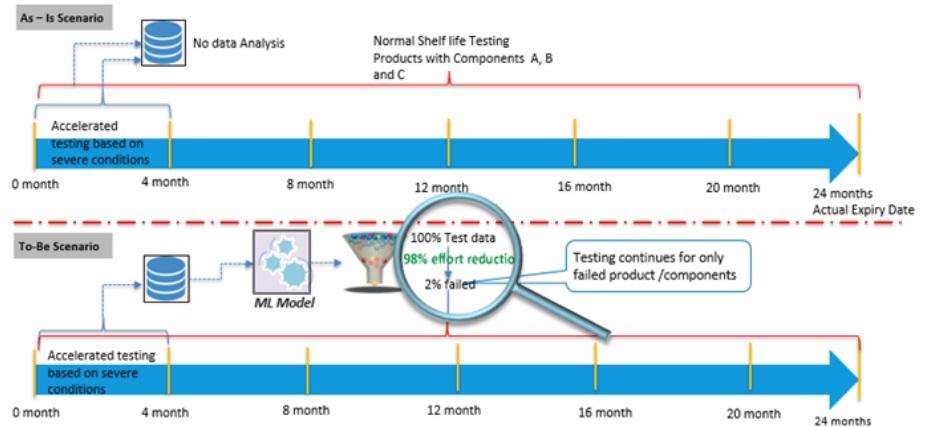
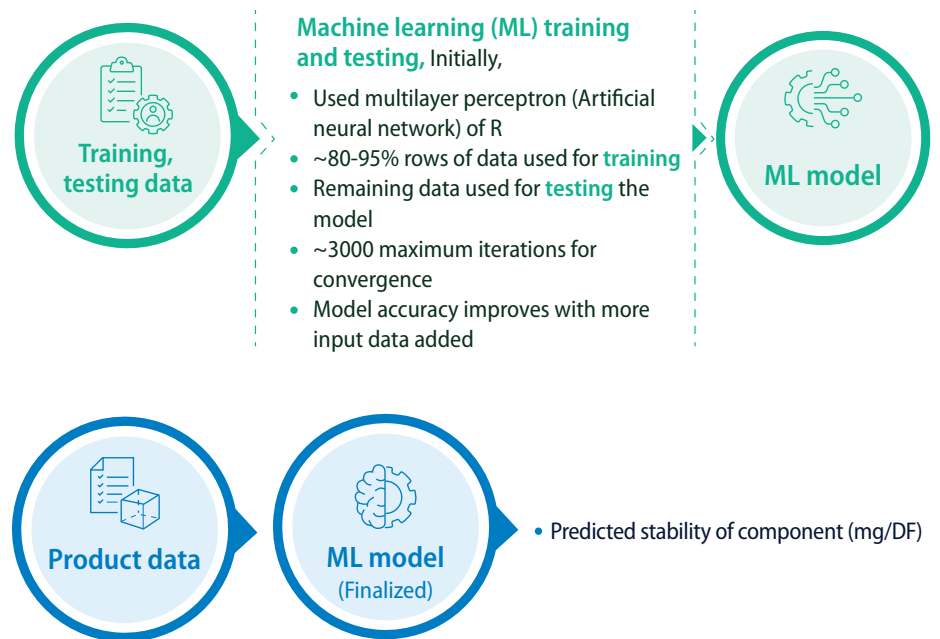


Figure 2 The ML process



## Approach

Product stability is influenced by various parameters such as its ingredients, test conditions (temperature, relative humidity), packaging type (bottle/blister), protocol (base/side/vertical) and period of measuring the stability. Hence these parameters become inputs for the machine learning model with stability as the output.

Models based on Artificial Neural Network (ANN) with implementation done in R language using MonMLP package and RShiny web interface give robust results. The model training was done using historical data with nearly 300 product IDs. The robustness of the model enables the inclusion of other influencing parameters such as microbiological characteristics in the future.



## Prediction Model

Description: The user (in the design phase) can experiment or simulate 'what if' scenarios by changing the proportions of ingredients. For new material composition, the stability is predicted to check if the product is stable after 24 -26 months.

Result/Value Addition: Prediction of product stability for different concentration levels and/or different combinations.

Figure 3 Stability of X Drug, with increase of ingredients concentration

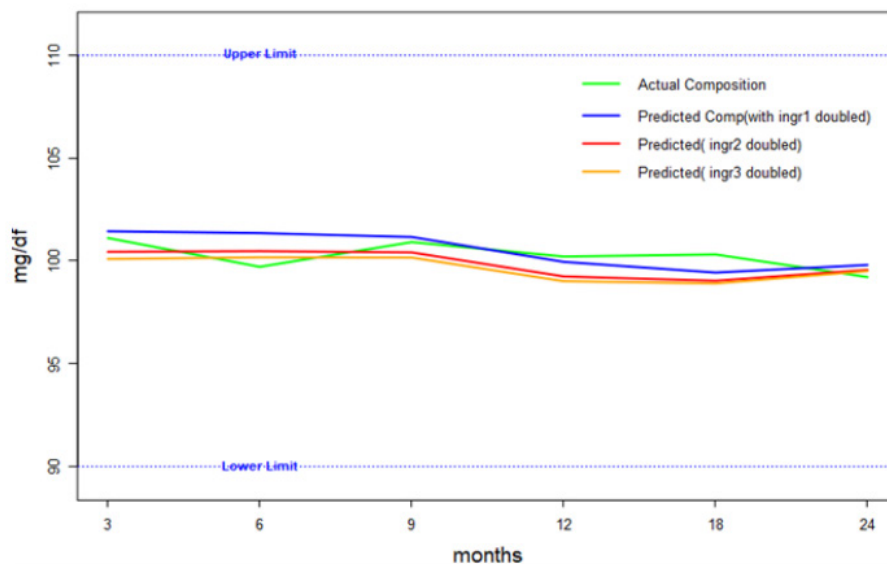
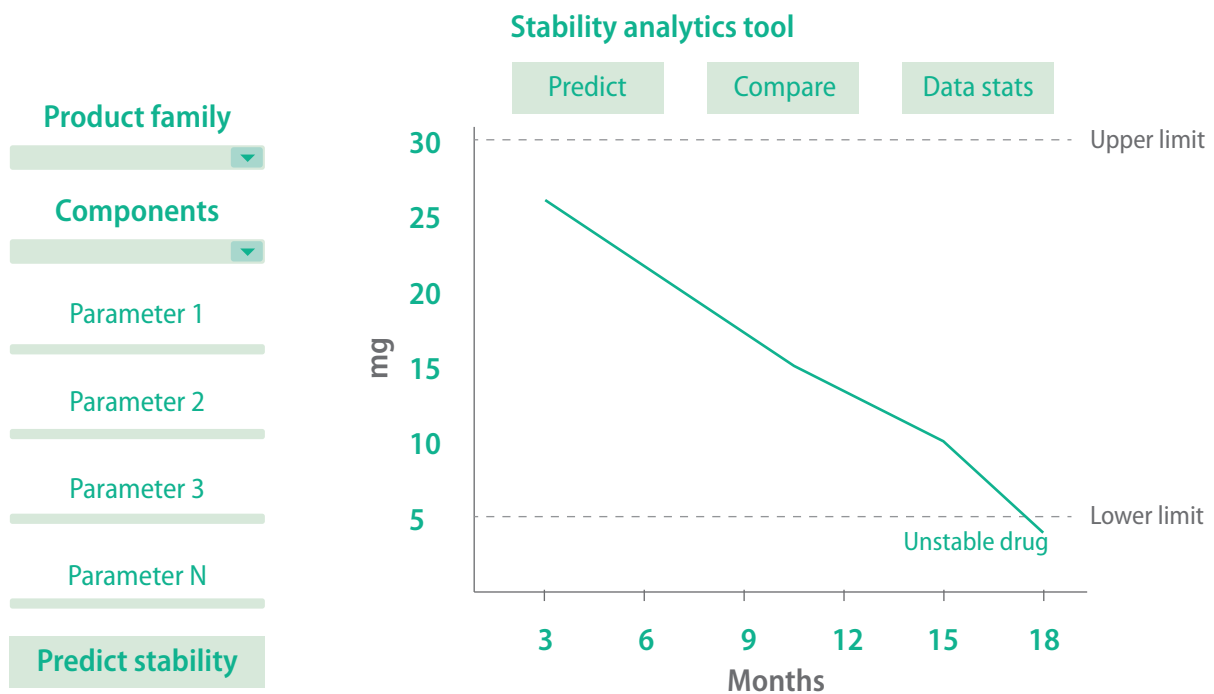




Figure 4 Glimpse of the stability prediction tool



## Tool Capabilities

- A visual presentation of the actual prediction curve
- Compare various stability values in the same product family
- Change temperature and relative humidity, set upper and lower limits, and time series
- Provide the source data and accuracy of the prediction
- Reporting features

## Business Drivers



### Reduce time of test

The model predicts the stability value of the component and is classified as pass or fail based on where it lies in a predefined range. So, testing must be conducted only for failed components, while testing time and efforts will be saved for passed components.



### Optimum resource utilization

Using stability analytics eliminates the need to conduct traditional testing on products predicted as passed by the model thus resulting in time and cost savings.



### Higher visibility about the product shelf life

Stability analytics help the user know the stability value predicted by the model at the required time point, which in turn will help determine the product shelf life faster.



### Study the effect of product design/ recipe changes on the stability of the product

The user will be able to select parameters like state, component, temperature and humidity through the filters provided, which will help get a better understanding of how the stability value changes with change in these parameters.



### Helps in root cause analysis of any product related failures

It lets the user experiment with different combinations of ingredients and conditions to determine its impact on the stability value which helps arrive at the root cause of the product failure.

## Business Benefits

- **Faster time to market:** Pharma companies spend considerable time testing their products which delays the entry of the product into the market. Using stability analytics will shorten the testing time and enable the company to launch the product sooner.
- **Saving resources involved in testing:** The stability analytical model helps the company save time, cost and other resources involved in performing traditional testing for all components as the model predicts pass or fail for the components. So, testing must be conducted only on failed components to determine the product shelf life.
- **Helps development team decide the appropriate combination of ingredients:** Enables development team members to know the impact of ingredients and conditions on

the final product before the start of the production phase.

- **Future Drug Development:** Any future variants in the drug can be understood and helps arrive at a go/no-go decision
- **Scalable Solution:** Solution is applicable across industries like Pharma, CPG and Cosmetics.

## Use cases

### 1. Optimize QC lab resources as normal shelf life testing only for components that do not follow the ML model output

The user, a lab technician, gets to know stability results predicted by the model just with a click. Thereby, long-term testing can be avoided/minimized for many components. Here, traditional testing must be done only for components that have been predicted as failed by the model. Again, this reduces time and saves resources.

### 2. Product development team to understand the stability of various ingredients and their combination/percentage

The user (in the design phase) can experiment/simulate 'what if' scenarios by changing the proportions of ingredients. For new material composition, stability is predicted to check if the product is stable after a specific number of months. This helps the user in the development team get the prediction on product stability for different concentration levels and/or different combinations.

## Take Away

Infosys Stability Analytics tool can optimize efforts for new drug variant discovery and ease out the decision making process by utilizing past data and predicting any unforeseen future road blocks during the R&D phase.

## Authors

### Amit Shriram Galgale

*Infosys - Principal Consultant, IOT*

20 years experience in Life Sciences, Pharma IOT, Analytics,  
IT Regulatory and Compliance, MES

### Satyanarayana k

*Infosys – Principal Consultant Advanced Engineering Group*

30 years of experience in Advanced Engineering, Data  
Analytics, AI and ML

For more information, contact [askus@infosys.com](mailto:askus@infosys.com)



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