

# PI World 2019 Lab

*Advanced Analytics and Machine Learning Use Cases  
with Industrial Sensor Data*



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**Data Science – Advanced Analytics and Machine Learning Use Cases – Hands-on Lab – OSIsoft PI World 2019**

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# Advanced Analytics and Machine Learning Use Cases with Industrial Sensor Data

## Lab Description

In previous years, we have explored the use of advanced analytics and machine learning for:

>Anomaly detection in an HVAC air-handler - [more](#)

>RUL (remaining useful life) prediction based on engine operations and failure data - [more](#)

>Golden-run identification for the temperature profile from a feed dryer (silica gel/molecular sieve) in an oil refinery - [more](#)

Additionally, as part of the above labs, we have used analytical methods such as PCA (principal components), SVM (support vector), shape similarity measures etc. And, in other similar labs, we have covered well-known algorithms for regression, classification etc. and reviewed the use of Azure Machine Learning - [more](#) - and open source platforms such as R and Python.

In this year's lab, we explore the use of historical process data to predict quality and yield for a product (Yeast) in batch manufacturing. We'll use multivariate [PCA](#) modeling to walk-through the diagnostics for monitoring the 14-hour evolution of each batch. And, alert you when a batch may go "bad" as critical operating parameters violate "golden batch" criteria ((high pH, low Molasses etc.). And, then we utilize [PLS](#) – projection to latent structures - to predict product quality and yield at batch completion.

The lab illustrates the end-to-end tasks in a typical data science project – from data preparation, conditioning, cleansing etc. to model development using training data, testing/validation using unseen data, and finally, deployment for production use with real-time data.

The techniques explored in the lab are not limited to batch manufacturing; they can be applied to several industries and to numerous processes that are multivariate in nature.

No coding or prior experience with [open source R](#) or [Python](#) is necessary but familiarity with the PI System is a pre-requisite.

Who should attend? Power User and Intermediate

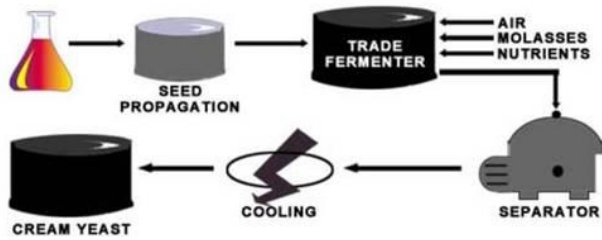
Duration: 3 hours

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## Summary

In this lab, we review [Yeast manufacturing](#) operations – specifically, the fermentation process. A typical batch of yeast fermentation takes 13 to 14 hours. There are many variables that can affect the yield and

quality of a batch: feed variability (molasses, air, NH3), byproducts (ethanol), bioreactor conditions (temperature, pH). Any combination of these factors can result in “bad” batch runs.



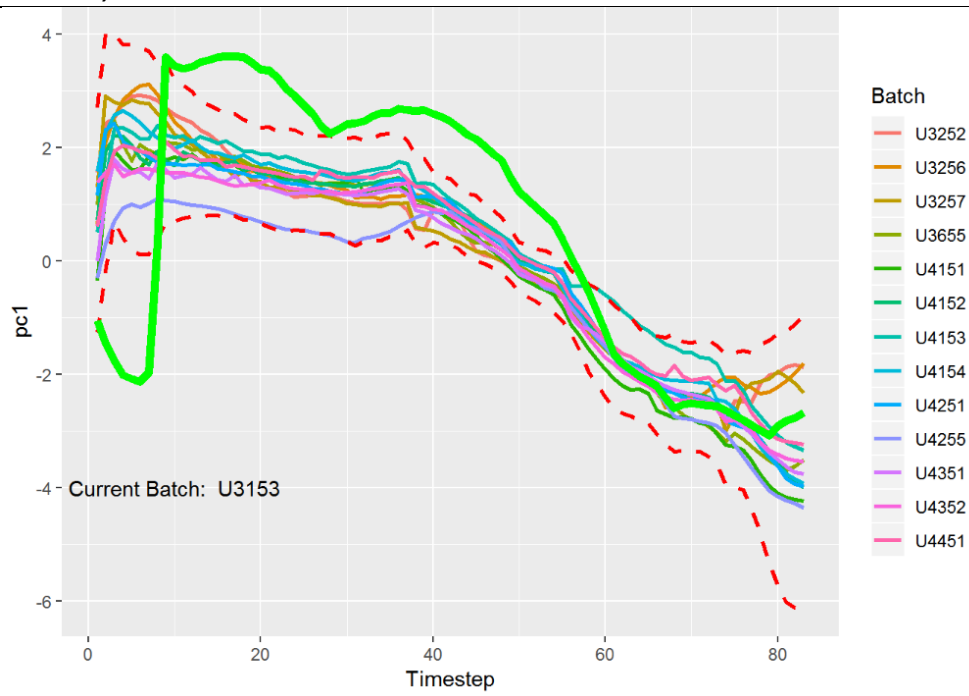
We want to use historic operations data with known “good” runs as a basis for alerts when current production parameters deviate from “golden batch” conditions. We also want to predict quality parameters, generically referred as QP1 and QP2, and the expected yield for each batch.

Bioreactor					
<div>General</div> <div>Child Elements</div> <div>Attributes</div> <div>Ports</div> <div>Analyses</div> <div>Notification Rules</div> <div>Version</div>					
Filter					
		Name	Value	Time Stamp	Description
Category: Batch Info					
		Batch	None	3/5/2019 12:00:00 AM	Batch ID
		Batch Active	No	3/5/2019 12:00:00 AM	Active Fermentation Indicator
		Status	Good	3/4/2019 11:30:00 PM	Batch Status : Manual Entry from Operator
Category: Lab Data					
		Amount	5977 kg	3/4/2019 11:30:00 PM	Mass of yeast in bioreactor
		Innoc	973 g	3/4/2019 11:30:00 PM	Mass of Yeast in Inoculation
		QP1	91	3/4/2019 11:30:00 PM	Quality Parameter 1
		QP2	80	3/4/2019 11:30:00 PM	Quality Parameter 2
		Yield	0.5 %	3/4/2019 11:30:00 PM	Yield of fermentation
Category: Process Data					
		Air	0 m3/h	3/5/2019 12:00:00 AM	Air Flowrate
		Ethanol	0 mg/L	3/5/2019 12:00:00 AM	Ethanol Concentration
		Level	0 %	3/5/2019 12:00:00 AM	Bioreactor Level
		Molasses	0 m3/h	3/5/2019 12:00:00 AM	Molasses Flowrate
		NH3	0 L/h	3/5/2019 12:00:00 AM	NH3 Flowrate
		pH	7	3/5/2019 12:00:00 AM	Bioreactor pH
		Temp	25 °C	3/5/2019 12:00:00 AM	Bioreactor Temperature

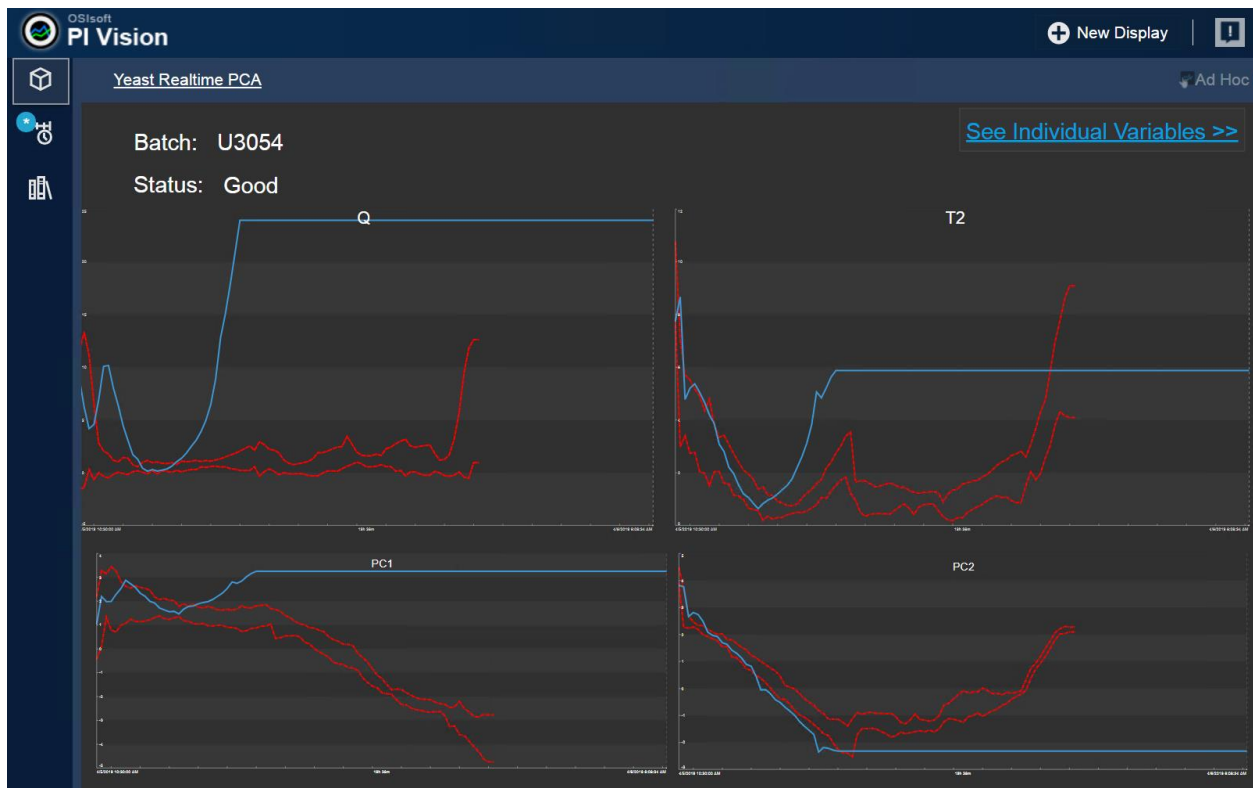
### Exercise 1: Monitoring the batch evolution

In this Exercise, we will use PCA model to develop the multivariate metrics to monitor the evolution of the batch as it is running and alert when conditions deviate from the model defined 3-sigma limits.

## Summary

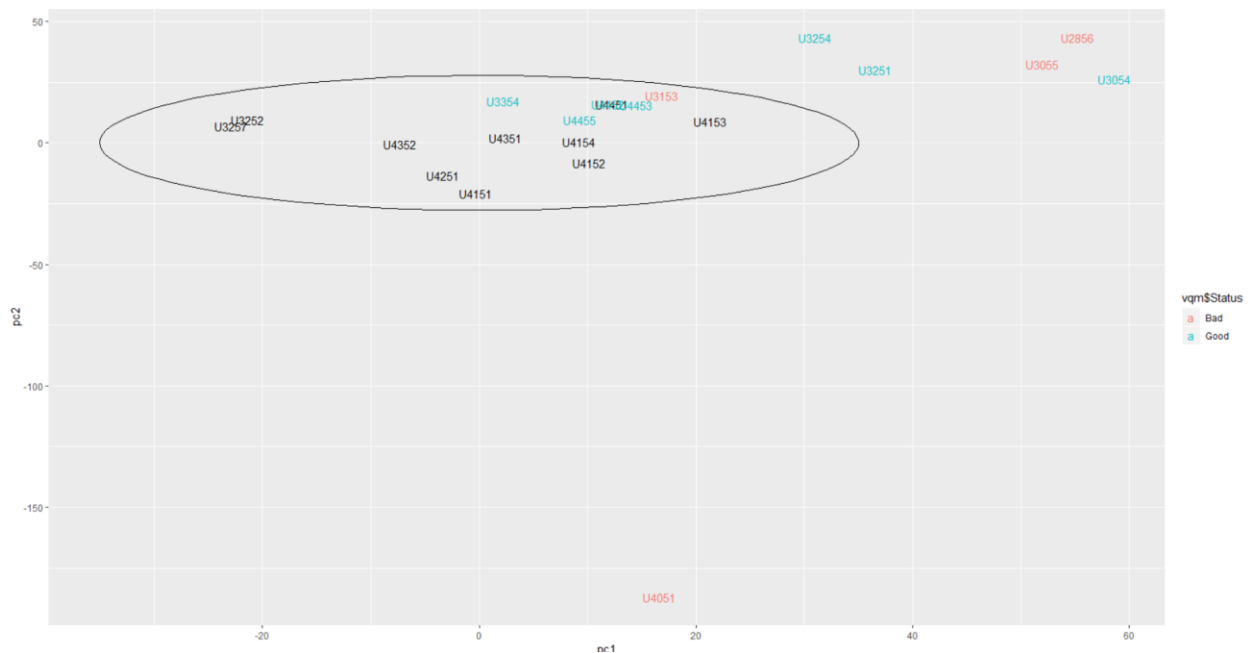


Add a new variable		Evaluate
Name	Expression	Output Attribute
BatchAct	'Batch Active' = 1	Map
PC1var	If BatchAct Then ('Ethanol'-(0.6546))/0.4914*0.3986+('Temp'-(31.16))/1.226*-0.4698+('Molasses'-(2136))/957.1*-0.06959+('NH3'-(107.5))/63.6*0.336+('Air'-(5872))/1444*-0.3142+('Level'-(48.63))/5.067*-0.5222+('pH'-(5.205))/0.3461*-0.3622 Else DigState("No Data")	PC1
PC2var	If BatchAct Then ('Ethanol'-(0.6546))/0.4914*-0.1048+('Temp'-(31.16))/1.226*0.1278+('Molasses'-(2136))/957.1*-0.06959+('NH3'-(107.5))/63.6*0.336+('Air'-(5872))/1444*-0.3142+('Level'-(48.63))/5.067*-0.5222+('pH'-(5.205))/0.3461*-0.3622 Else DigState("No Data")	PC2
T2var	//Hotelling T2 If BatchAct Then (PC1var/1.836)^2+(PC2var/1.402)^2 Else DigState("No Data")	T2



## Exercise 2: Full batch assessment

In this Exercise, we will use the full batch run data – with PCA to make an assessment regarding “good” vs. “bad” batch. This is useful when the results from lab quality analysis may not be available for 4-8 hours after the end of a batch.

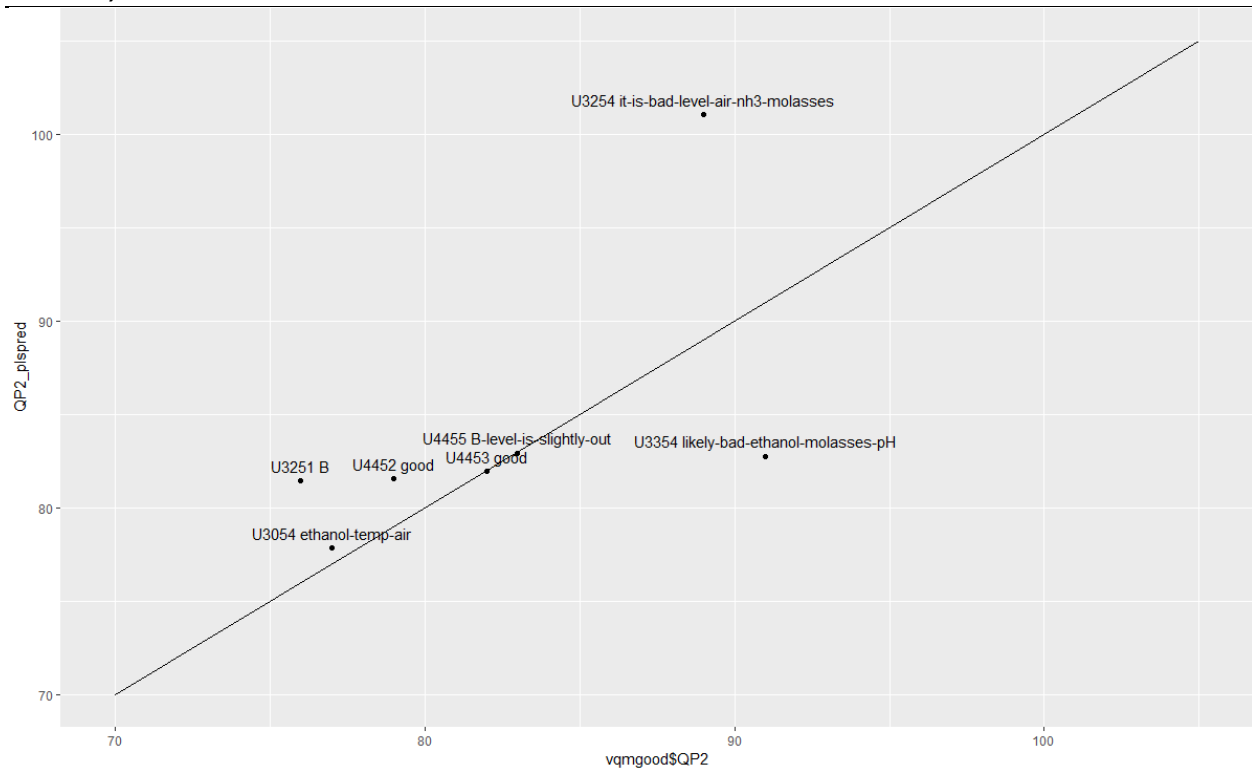


## Exercise 3: Predict quality

In the portion of the lab, we will use PLS to predict quality.



## Summary



## Installed Software

### PI System

The VM (virtual machine) used for this lab has the following PI System software installed:

Software	Version
PI Data Archive	2018
PI Asset Framework (PI AF) server	2018
PI Asset Framework (PI AF) client (PI System Explorer)	2018
PI Analysis & PI Notifications Services	2018
PI Vision	2017 R2 SP1
PI Web API	2018
PI Integrator for Business Analytics	2018 R2

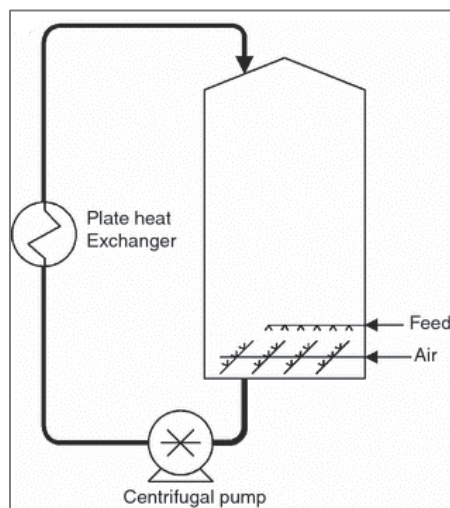
For details on PI System software, please refer to:

<http://www.osisoft.com/pi-system/pi-capabilities/product-list/>

## Part I – Explore Yeast Manufacturing Operations and Extract Data using PI Integrator

### Process Description

We have a plant manufacturing Baker's yeast in a fed-batch bioreactor with a circulation loop, shown below.



- Air is supplied via an air sparger, and mixing ensures tank aeration.
- Molasses is fed using perforated pipes at the bottom of the bioreactor.
- Ethanol concentration is monitored using an in-line sensor.
- Acidity in the bioreactor is monitored using a pH sensor in the circulation loop.
- A plate heat exchanger is used to control temperature, which is monitored using a thermocouple.
- Bioreactor level is also monitored via a sensor.
- All process signals described above are transmitted to a programmable logic controller (PLC)
- The operator enters the Batch ID, and whether the batch is "Active" in the PLC through a Human Machine Interface (HMI). They can also manually enter if the batch has been "Good" or "Bad" at the end of the batch.

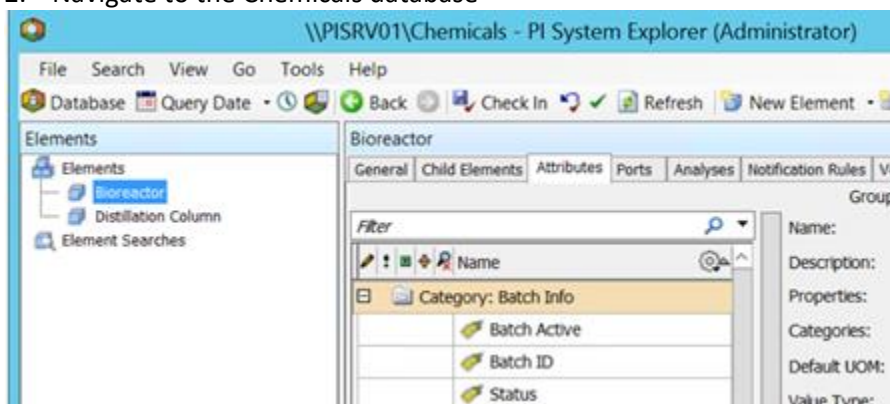
At the beginning of the batch, a sample of the inoculum is sent to the lab. When the batch is completed, samples of the bioreactor broth are taken for analysis. Lab data is measured and/or calculated for each batch, and entered in the laboratory information management system (LIMS). This includes:

- The mass of yeast in the inoculum
- The final amount of yeast in the bioreactor
- The yield
- Two additional quality parameters, referred generically as QP1 and QP2

## Step 1: Explore the AF model

An AF model has already been created for the yeast production process.

1. Run PI System Explorer
2. Navigate to the Chemicals database



3. Select “Bioreactor”, and navigate to the “Attributes” tab.

Bioreactor

General

Child Elements

Attributes





















Ports

Analyses

Notification Rules

Version

Filter

    	Name	Value	Time Stamp	Description
Category: Batch Info				
	 Batch	None	3/5/2019 12:00:00 AM	Batch ID
	 Batch Active	No	3/5/2019 12:00:00 AM	Active Fermentation Indicator
	 Status	Good	3/4/2019 11:30:00 PM	Batch Status : Manual Entry from Operator
Category: Lab Data				
	 Amount	5977 kg	3/4/2019 11:30:00 PM	Mass of yeast in bioreactor
	 Innoc	973 g	3/4/2019 11:30:00 PM	Mass of Yeast in Inoculation
	 QP1	91	3/4/2019 11:30:00 PM	Quality Parameter 1
	 QP2	80	3/4/2019 11:30:00 PM	Quality Parameter 2
	 Yield	0.5 %	3/4/2019 11:30:00 PM	Yield of fermentation
Category: Process Data				
	 Air	0 m3/h	3/5/2019 12:00:00 AM	Air Flowrate
	 Ethanol	0 mg/L	3/5/2019 12:00:00 AM	Ethanol Concentration
	 Level	0 %	3/5/2019 12:00:00 AM	Bioreactor Level
	 Molasses	0 m3/h	3/5/2019 12:00:00 AM	Molasses Flowrate
	 NH3	0 L/h	3/5/2019 12:00:00 AM	NH3 Flowrate
	 pH	7	3/5/2019 12:00:00 AM	Bioreactor pH
	 Temp	25 °C	3/5/2019 12:00:00 AM	Bioreactor Temperature

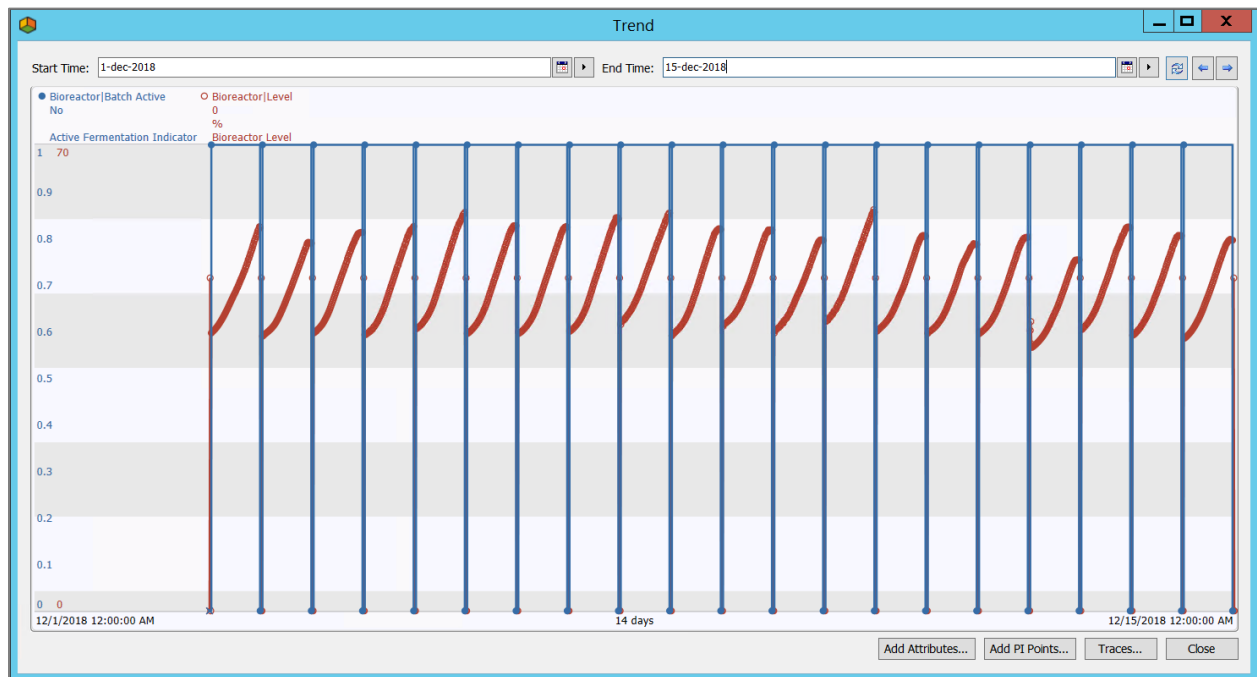
The attributes under “Batch Info” and “Process Data” are collected in near real-time. The “Lab Data” is collected by the LIMS where the lab sample uses the batch end timestamp for the lab results.

## Step 2: Explore yeast batch Event Frames

We use asset analytics to generate the Event Frames needed to analyze yeast batch data.

1. In the Bioreactor element, navigate to “Attributes” tab
2. While holding the CTRL key, select the “Batch Active” and “Level” attributes
3. Right-click and select “Trend”
4. Change the start time to 1-dec-2018 and the end time to 15-dec-2018

You should see the following trend:



In the trend, the “Batch Active” value is “Yes”, an active batch is running and hence it is used to generate the Event Frames.

1. Close the trend window
2. Navigate to the “Analyses” tab
3. Review the “Yeast Batch” Event Frame Generation Analysis.

Generation Mode:  Event Frame Template:

A transition from zeroth state to any other state starts an event frame, and transition to the zeroth state ends the event frame

Triggering Input:

Zeroth States:




















































Advanced Event Frame Settings...

In the “Pulse” generation mode, by setting the Triggering Input to “Batch Active”, and Event Frame will be created when the value changes to “Yes”, and will close when the value changes to “No”.

















To see the end result:

1. Navigate to the Event Frames tab
2. Right-click on “Event Frame Searches” and select “New Search”
3. In the Event Frame Search Window, select the Template “Yeast Batch” and click OK

You will see several Event Frames:

Yeast Batches						
Filter						
   Name	Duration	Start Time	Batch	Status	Amount	
  U2952 - Yeast Batch	13:40:00	12/3/2018 1:30:00 AM	U2952	No Data	No Data	
  U2953 - Yeast Batch	13:40:00	12/3/2018 3:50:00 PM	U2953	No Data	No Data	
  U3152 - Yeast Batch	13:40:00	12/4/2018 6:10:00 AM	U3152	Bad	6368 kg	
  U3252 - Yeast Batch	13:40:00	12/4/2018 8:30:00 PM	U3252	Good	6658 kg	
  U3253 - Yeast Batch	13:40:00	12/5/2018 10:50:00 AM	U3253	No Data	No Data	
  U3256 - Yeast Batch	13:40:00	12/6/2018 1:10:00 AM	U3256	Good	7120 kg	
  U3257 - Yeast Batch	13:40:00	12/6/2018 3:30:00 PM	U3257	Good	6920 kg	
  U3351 - Yeast Batch	13:40:00	12/7/2018 5:50:00 AM	U3351	No Data	No Data	
  U3451 - Yeast Batch	13:40:00	12/7/2018 8:10:00 PM	U3451	No Data	No Data	
  U3655 - Yeast Batch	13:40:00	12/8/2018 10:30:00 AM	U3655	Good	6597 kg	
  U4151 - Yeast Batch	13:40:00	12/9/2018 12:50:00 AM	U4151	Good	5541 kg	
  U4251 - Yeast Batch	13:40:00	12/9/2018 3:10:00 PM	U4251	Good	5749 kg	
  U4255 - Yeast Batch	13:40:00	12/10/2018 5:30:00 AM	U4255	Good	5365 kg	
  U4152 - Yeast Batch	13:40:00	12/10/2018 7:50:00 PM	U4152	Good	5875 kg	
  U4153 - Yeast Batch	13:40:00	12/11/2018 10:10:00 AM	U4153	Good	5835 kg	
  U4154 - Yeast Batch	13:40:00	12/12/2018 12:30:00 AM	U4154	Good	5973 kg	
  U4155 - Yeast Batch	13:40:00	12/12/2018 2:50:00 PM	U4155	Bad	5402 kg	
  U4351 - Yeast Batch	13:40:00	12/13/2018 5:10:00 AM	U4351	Good	5982 kg	
  U4352 - Yeast Batch	13:40:00	12/13/2018 7:30:00 PM	U4352	Good	5977 kg	
  U4451 - Yeast Batch	13:40:00	12/14/2018 9:50:00 AM	U4451	Good	5977 kg	
  U2856 - Yeast Batch	13:40:00	2/28/2019 5:50:00 AM	U2856	Bad	5715 kg	
  U2954 - Yeast Batch	13:40:00	2/28/2019 8:10:00 PM	U2954	No Data	No Data	
  U3054 - Yeast Batch	13:40:00	3/1/2019 10:30:00 AM	U3054	Good	6089 kg	
  U3055 - Yeast Batch	13:40:00	3/2/2019 12:50:00 AM	U3055	Good	5904 kg	

Double-click on an Event Frame, and navigate to the “Attributes” tab.

U4255 - Yeast Batch				
General		Child Event Frames	Referenced Elements	Attributes
Filter				
	  	Name	Value	Time Stamp
Category: Batch Info				
<input checked="" type="checkbox"/>		Batch	U4255	2/28/2019 5:30:00 AM
<input checked="" type="checkbox"/>		Status	Good	2/28/2019 7:10:00 PM
Category: Lab Data				
<input checked="" type="checkbox"/>		Amount	5365 kg	2/28/2019 7:10:00 PM
<input checked="" type="checkbox"/>		Innoc	914 g	2/28/2019 7:10:00 PM
<input checked="" type="checkbox"/>		QP1	93	2/28/2019 7:10:00 PM
<input checked="" type="checkbox"/>		QP2	77	2/28/2019 7:10:00 PM
<input checked="" type="checkbox"/>		Yield	0.48 %	2/28/2019 7:10:00 PM
Category: Process Data				
<input checked="" type="checkbox"/>		Max Ethanol	0.85934 mg/L	2/28/2019 12:30:00 PM
<input checked="" type="checkbox"/>		Max pH	6.9551	2/28/2019 7:10:00 PM
<input checked="" type="checkbox"/>		Min pH	5.1592	2/28/2019 7:00:00 AM
<input checked="" type="checkbox"/>		Total Air	80328 m3	2/28/2019 7:10:00 PM
<input checked="" type="checkbox"/>		Total Molasses	33426 m3	2/28/2019 7:10:00 PM
<input checked="" type="checkbox"/>		Total NH3	1622.3 L	2/28/2019 7:10:00 PM

The attribute configuration in the “Yeast Batch” Event Frame template (found under Library) contains the lab data, and other process data aggregates.

Note that some batches have “No Data” under the Lab Data attributes. We may filter out these batches during analysis.

## Data Publication

Now that our batch data has been properly contextualized using Event Frames, we need to publish the historical data in a format suitable for multivariate modelling in R/Python.

Using PI Integrator for Business Analytics., we create two datasets:

- Training - data from **1 – 15 December 2018** for training and developing a model.
- Test - data from **28 February – 8 March** to test/validate the model.

For each dataset, we publish two tables:


- **Batch Summary table:** a table with initial conditions (inoculum) and final properties (quality, amount, yield) for each batch
- **Batch Evolution table:** a table that shows the evolution of the process data for the bioreactor (molasses, air, temperature, pH, ethanol). We will publish interpolated data at 10 minute intervals.

At the end of this step, you see 4 publications:

1. Training dataset – Batch Summary
2. Training dataset – Batch Evolution
3. Test dataset – Batch Summary
4. Test dataset – Batch Evolution

### Step 1: Training dataset – Batch Summary

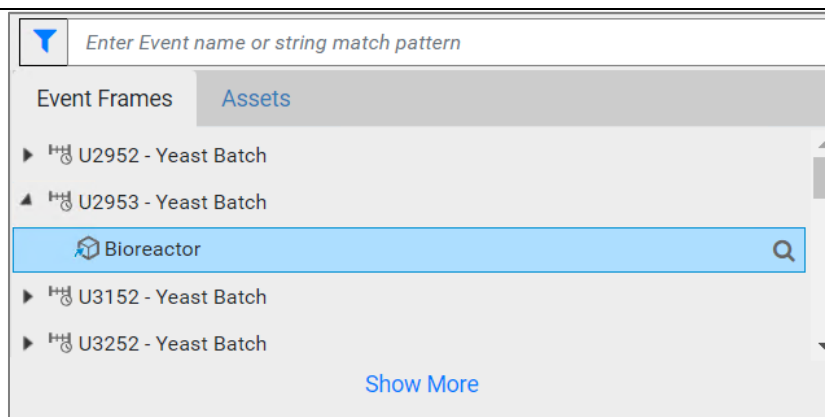
#### Select Data

1. Open Google Chrome and click on the “PI Integrator for BA” bookmark (<https://pisrv01:444/>).
2. Click on “Create Event View”.
3. Name the view “Modelling dataset – Batch Summary”.
4. Click on “Create a New Shape”.
5. On the Event View page, select the Database “Chemicals”.
6. Drag and drop on the of Yeast Batch Events into the event shape.
7. In the attributes pane at the bottom-left of the screen, press the sorting button  and select “Group by Category”.
8. Drag and Drop the “Batch Info” and “Lab Data” categories into the event shape.


Note: We will not bring in the “Process Data” attributes (e.g. Max Ethanol) in the event shape. The integrator does not support the “By Time Range” setting of Event Frame attributes. To get the Max Ethanol concentration, we will bring in the Bioreactor’s “Ethanol” attribute, and specify the aggregation needed in the next step.

9. In the Event Frames pane, expand the select event. You should see the “Bioreactor” element. Click on it:

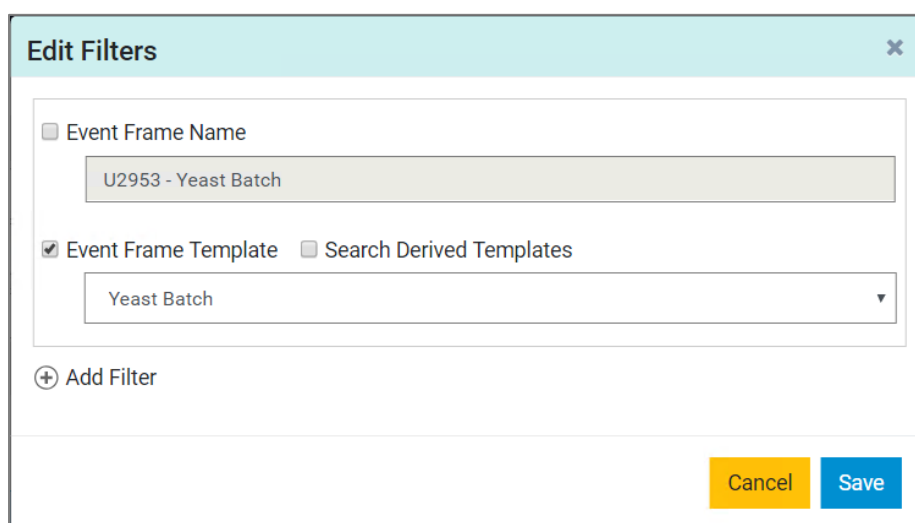




10. In the attributes pane at the bottom-left of the screen, drag and drop “Ethanol” into the event shape

11. Click on the edit button  next to the batch you dragged into the event shape.

12. Uncheck “Event Frame Name” and check “Event Frame Template”.

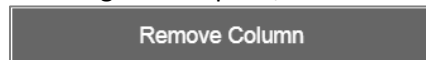


13. Your final result should look like the image below. If it does, click “Next”.

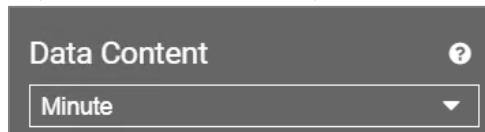
Search Shape	Matches
Event Shape	Found 13 Matches
Yeast Batch	U2856 - Yeast Batch
Amount	U2954 - Yeast Batch
Batch	U3054 - Yeast Batch
Innoc	U3055 - Yeast Batch
QP1	U3153 - Yeast Batch
QP2	U3251 - Yeast Batch
Status	U3254 - Yeast Batch
Yield	U3255 - Yeast Batch
Bioreactor	U3354 - Yeast Batch
Ethanol	U4051 - Yeast Batch
	U4452 - Yeast Batch
	U4453 - Yeast Batch
	U4455 - Yeast Batch

## Modify View

- On the “Modify View” page, change the start time to “1-dec-2018” and the end time to “15-dec-2018”
- Remove the “Timestamp” and “Bioreactor” columns
  - Select the column
  - In the right-hand pane, click the “Remove Column” button



- Change the “Event Frame Duration” Column from hours to minutes.
  - Select the column
  - In the right-hand pane, under “Data Content”, select “Minute”.



- Click “Apply Changes”
- For the “Ethanol” attributes, we must specify that we want to aggregate the data for the duration of the Event Frame.
    - Select the column
    - In the right-hand pane, under “Data Content”, select “Maximum”
    - Click “Apply changes”

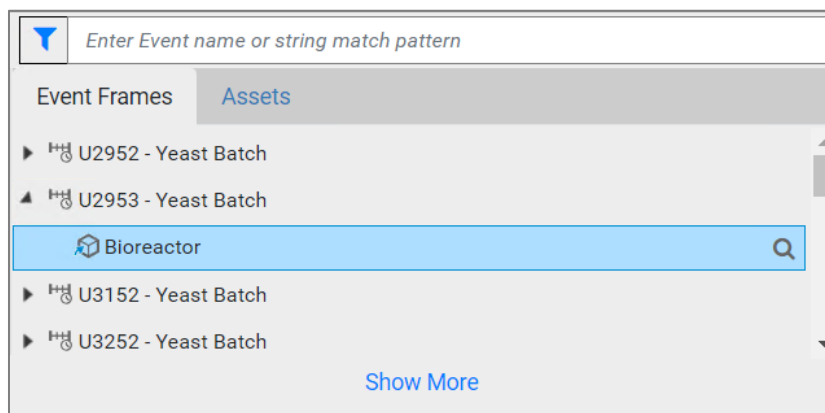
The data should look like the table below. If it does, click “Next”.



1. On the “Publish” page, under “Target Configuration” select the target named “CSV”
2. Leave the Run Mode as “Run Once”
3. Click “Publish”

## Step 2: Training dataset – Batch Evolution

### Select Data

1. On the PI Integrator homepage, click on “Create Event View”.
2. Name the view “Modelling dataset – Batch Summary”.
3. Click on “Create a New Shape”.
4. On the Event View page, select the Database “Chemicals”.
5. Select on the of Yeast Batch Events.
6. From the attributes pane, drag and drop the “Batch” attribute into the Event Shape.
14. In the Event Frames pane, expand the select event. You should see the “Bioreactor” element. Click on it:



7. In the attributes pane at the bottom-left of the screen, press the sorting button  and select “Group by Category”.
8. Drag and Drop the “Process Data” category into the Event Shape
9. Click on the edit button  next to the batch you dragged into the event shape.
10. Uncheck “Event Frame Name” and check “Event Frame Template”.

Edit Filters

☐ Event Frame Name
 

U2953 - Yeast Batch

☒ Event Frame Template
 ☐ Search Derived Templates
 

Yeast Batch

+

 Add Filter

Cancel

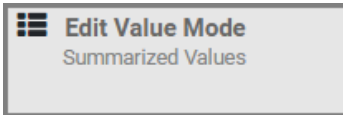
Save

11. Your final result should look like the image below. If it does, click “Next”.

Search Shape	Matches
<div>Event Shape</div> <div> <div>Yeast Batch</div> <div> <div>Batch</div> <div> <div>Bioreactor</div> <div>Air</div> <div>Ethanol</div> <div>Level</div> <div>Molasses</div> <div>NH3</div> <div>Temp</div> <div>pH</div> </div> </div> </div>	<div>Found 13 Matches</div> <div> <div>U2856 - Yeast Batch</div> <div>U2954 - Yeast Batch</div> <div>U3054 - Yeast Batch</div> <div>U3055 - Yeast Batch</div> <div>U3153 - Yeast Batch</div> <div>U3251 - Yeast Batch</div> <div>U3254 - Yeast Batch</div> <div>U3255 - Yeast Batch</div> <div>U3354 - Yeast Batch</div> <div>U4051 - Yeast Batch</div> <div>U4452 - Yeast Batch</div> <div>U4453 - Yeast Batch</div> <div>U4455 - Yeast Batch</div> </div>

### Modify View

1. On the “Modify View” page, change the start time to “1-dec-2018” and the end time to “15-dec-2018”
2. Remove the “Event Frame Start Time”, “Event Frame End Time” and “Duration” column



3. Click on “Edit Value Mode”
4. Select “Sample Values” and set “Sample values every 10 minutes”, with interpolation.

A dialog box titled "Edit Value Mode" with a close button (X) in the top right corner. The dialog contains several radio button options: "Summarized Values", "Sampled Values" (which is selected), "Interpolate" (with an information icon), "Exact" (with an information icon), and "Use Key Column" (with a dropdown menu showing "Batch"). Under "Sampled Values", there is a sub-option "Sample values every" followed by a dropdown menu showing "10" and another dropdown menu showing "minutes". At the bottom right of the dialog are two buttons: "Cancel" (yellow) and "Save Changes" (blue).

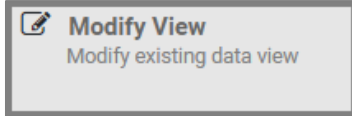
5. Click next.

### Publish

1. On the “Publish” page, under “Target Configuration” select the target named “CSV”
2. Leave the Run Mode as “Run Once”
3. Click “Publish”

### Step 3: Test dataset – Batch Summary

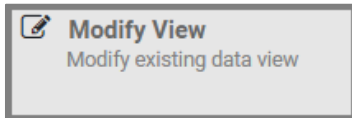
1. On the PI Integrator homepage, select the view you just created: “Modelling dataset – Batch Summary”.
2. Click “Modify View”



3. Select “Edit a copy of this View” and name it “Test dataset – Batch Summary”
4. On the “Select Data” page, click “Next”.
6. On the “Modify View” page, change the start time to “28-feb-2019” and the end time to “8-mar-2019”. Click “Next”
7. On the “Publish” page, click “Publish”

### Step 4: Test dataset – Batch Evolution

5. On the PI Integrator homepage, select the view you just created: “Modelling dataset – Batch Evolution”.
6. Click “Modify View”

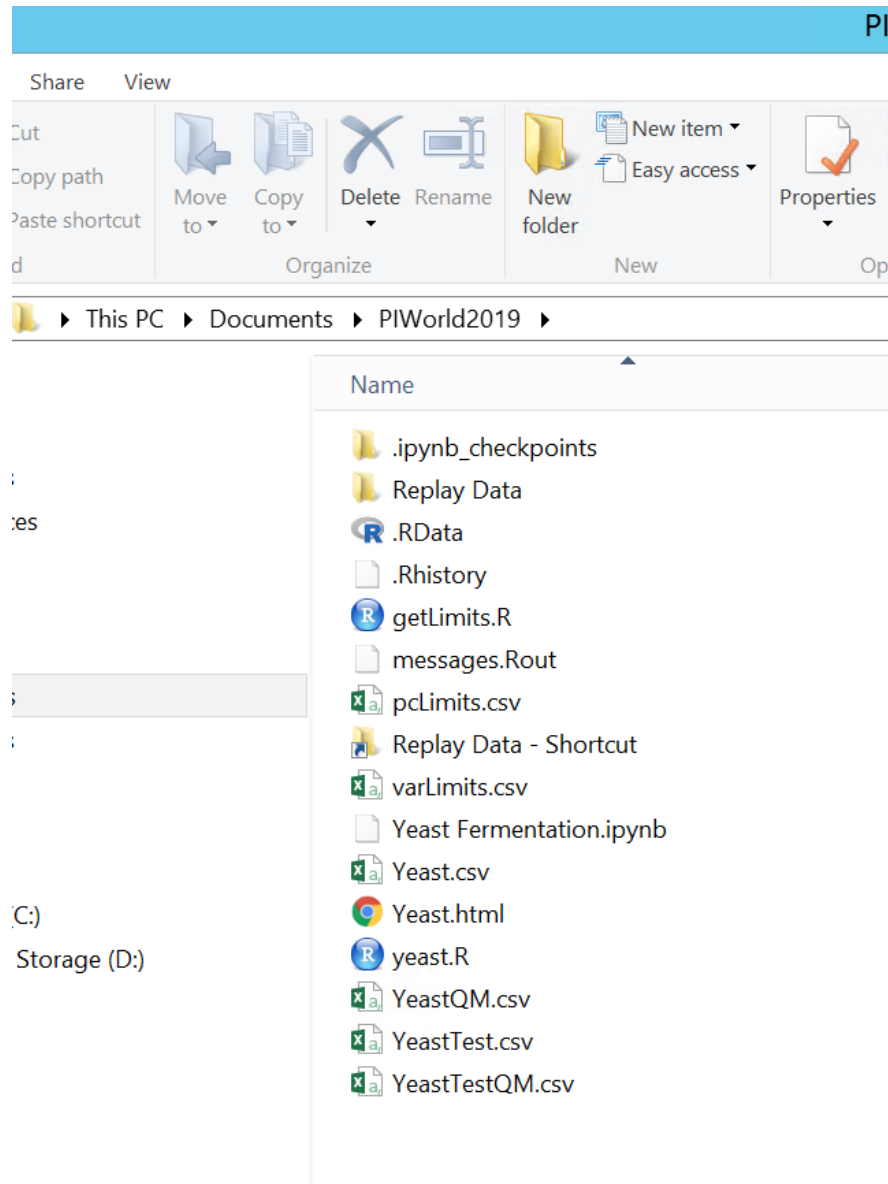


7. Select “Edit a copy of this View” and name it “Test dataset – Batch Evolution”
8. On the “Select Data” page, click “Next”.
8. On the “Modify View” page, change the start time to “28-feb-2019” and the end time to “8-mar-2019”. Click “Next”
9. On the “Publish” page, click “Publish”

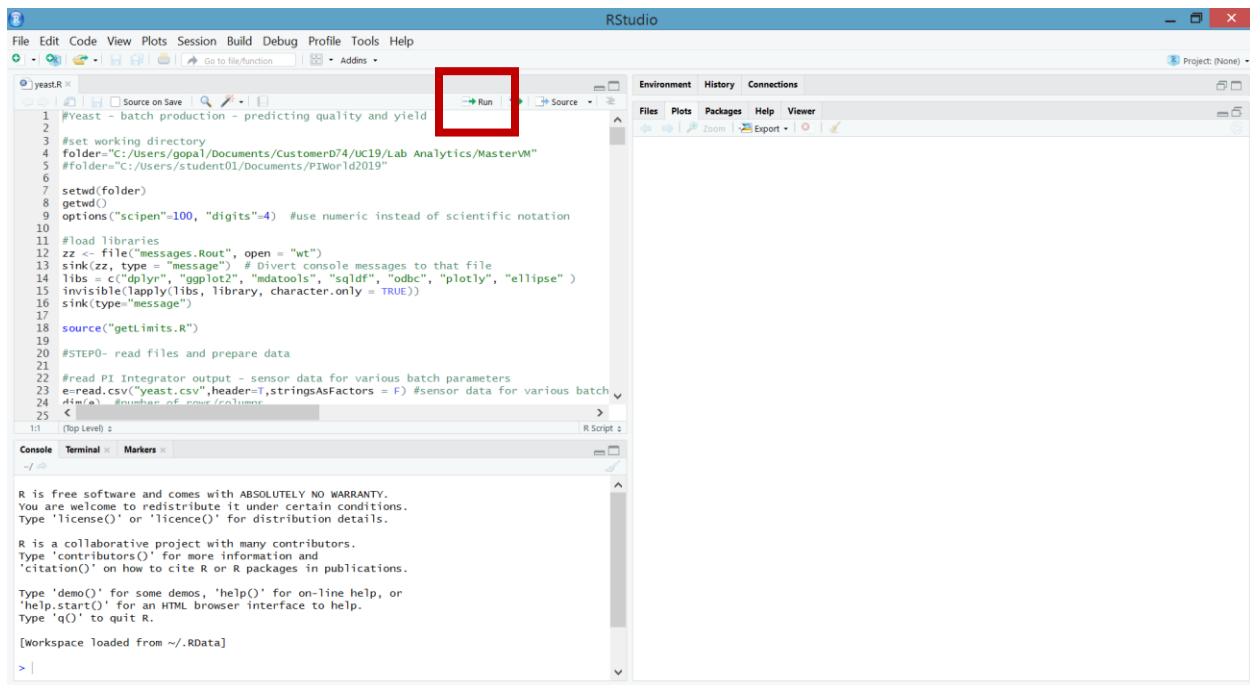
## Part II – Model Development Using R

### Exercise 1 – Monitoring the Batch Evolution

From the PIWorld2019 folder, select yeast.R and double-click to open it in R Studio (please be patient, R Studio takes a few seconds to open).

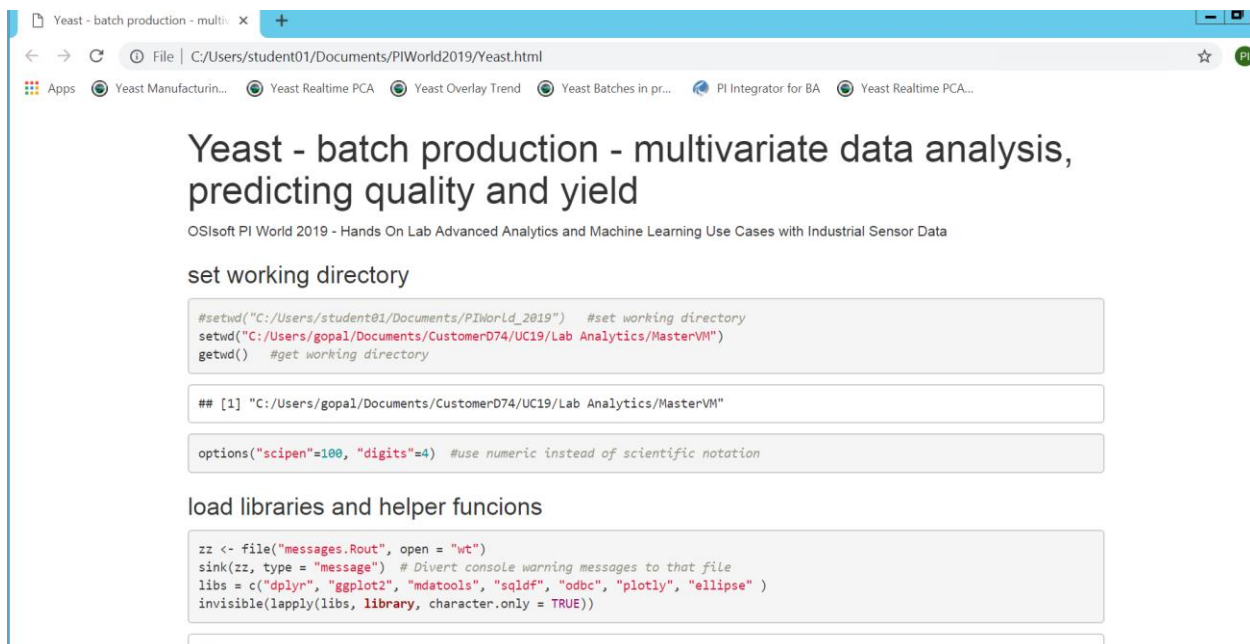


The screen below shows the R Studio user interface.



The output from the script as you run it line by line using **Run** is shown in Yeast.html (see the lab folder for the latest revision).

Only the first page from Yeast.html is shown below.



Please refer to the electronic copy of Yeast.html in the Lab VM.



## Part II - Model deployment and real-time scoring

### Step 1: AF Analytics

The relevant step from the R script is shown below (Step 1-5 in the R script output – html document)

#### Exercise 1 BATCH EVOLUTION #### STEP 1-5 deploy in AF Analytics

```
pc1eq="" #get pc1 equation
for (j in 1:7)
{pc1eq=cat(sep="",pc1eq,"+(", "",names(egood.pca$center[j]), "", "-(",egood.pca$center[j],"),",")/",egood.pca$scale[j], "*",ego
od.pca$loadings[j,1])}
```

```
## +('Ethanol'-(0.6546))/0.4914*0.3986+('Temp'-(31.16))/1.226*-0.4698+('Molasses'-(2136))/957.1*-0.06959+('NH3'-(107.5))/63.
6*0.336+('Air'-(5872))/1444*-0.3142+('Level'-(48.63))/5.067*-0.5222+('pH'-(5.205))/0.3461*-0.3622
```

```
pc2eq="" #get pc2 equation
for (j in 1:7)
{pc2eq=cat(sep="",pc2eq,"+(", "",names(egood.pca$center[j]), "", "-(",egood.pca$center[j],"),",")/",egood.pca$scale[j], "*",ego
od.pca$loadings[j,2])}
```

```
## +('Ethanol'-(0.6546))/0.4914*-0.1048+('Temp'-(31.16))/1.226*0.1278+('Molasses'-(2136))/957.1*-0.6414+('NH3'-(107.5))/63.6
*-0.5026+('Air'-(5872))/1444*-0.5366+('Level'-(48.63))/5.067*-0.1381+('pH'-(5.205))/0.3461*0.04061
```

```
#T2 equation
T2eq=""
T2eq=cat(sep="", '(pc1/',sd(egood.pca$calres$scores[,1]),')^2+(pc2/', sd(egood.pca$calres$scores[,2]),')^2')
```

```
## (pc1/1.836)^2+(pc2/1.402)^2
```

```
#Q equation
Qeq=""
for (j in 1:7)
{Qeq=cat(sep="",Qeq,"+(", "",names(egood.pca$center[j]), "", "-(",egood.pca$center[j],"),",")/",egood.pca$scale[j], "-(", "PC1Var
*",egood.pca$loadings[j,1],"+PC2Var*",egood.pca$loadings[j,2],")^2")}
```

```
## +(((('Ethanol'-(0.6546))/0.4914-(PC1Var*0.3986+PC2Var*-0.1048))^2+((('Temp'-(31.16))/1.226-(PC1Var*-0.4698+PC2Var*0.1278))^2
+((('Molasses'-(2136))/957.1-(PC1Var*-0.06959+PC2Var*-0.6414))^2+(((('NH3'-(107.5))/63.6-(PC1Var*0.336+PC2Var*-0.5026))^2+((('Ai
r'-(5872))/1444-(PC1Var*-0.3142+PC2Var*-0.5366))^2+((('Level'-(48.63))/5.067-(PC1Var*-0.5222+PC2Var*-0.1381))^2+((('pH'-(5.20
5))/0.3461-(PC1Var*-0.3622+PC2Var*0.04061))^2
```

### Step 2: (Optional) Copy/paste the equations from R to AF Analytics

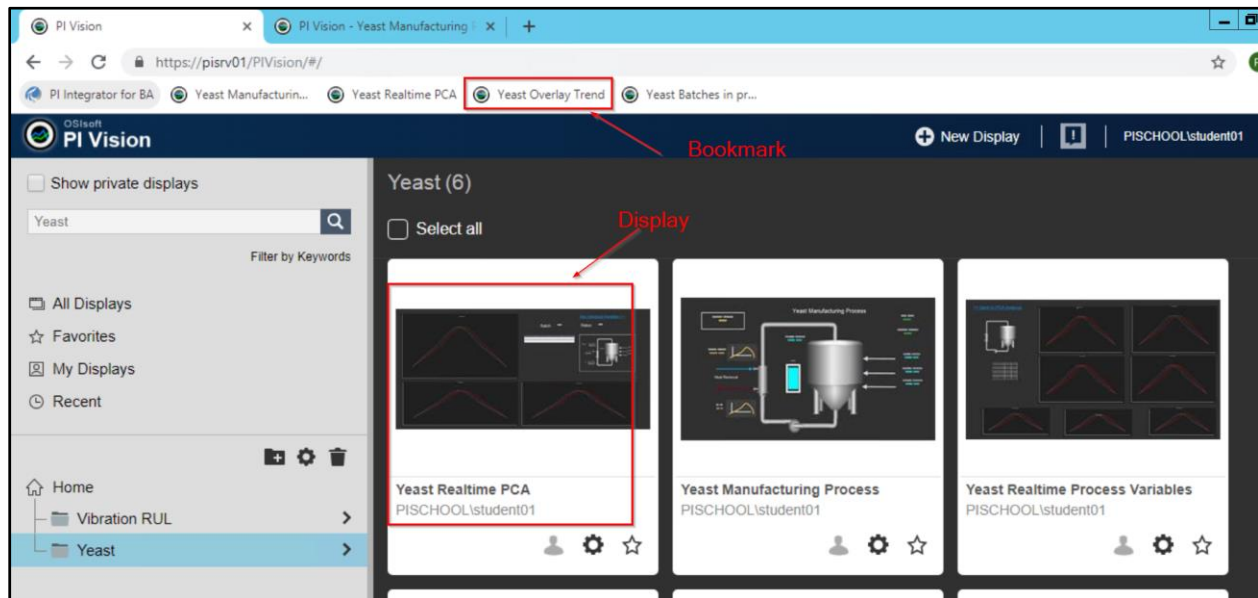
Add a new variable		↑	↓	Evaluate
Name	Expression	Output Attribute		
BatchAct	'Batch Active' = 1	Map		
PC1var	If BatchAct Then ('Ethanol'-(0.6546))/0.4914*0.3986+('Temp'-(31.16))/1.226*-0.4698+('Molasses'-(2136))/957.1*-0.06959+('NH3'-(107.5))/63.6*0.336+('Air'-(5872))/1444*-0.3142+('Level'-(48.63))/5.067*-0.5222+('pH'-(5.205))/0.3461*-0.3622 Else DigState("No Data")	PC1		
PC2var	If BatchAct Then ('Ethanol'-(0.6546))/0.4914*-0.1048+('Temp'-(31.16))/1.226*0.1278+('Molasses'-(2136))/957.1*-0.6414+('NH3'-(107.5))/63.6*-0.5026+('Air'-(5872))/1444*-0.5366+('Level'-(48.63))/5.067*-0.1381+('pH'-(5.205))/0.3461*0.04061 Else DigState("No Data")	PC2		
T2var	//Hotelling T2 If BatchAct Then (PC1var/1.836)^2+(PC2var/1.402)^2 Else DigState("No Data")	T2		

### Step 3: Real-time scoring



To mimic the user experience during an actual batch production run, replay the data from one of the batches (U3054) as shown below.

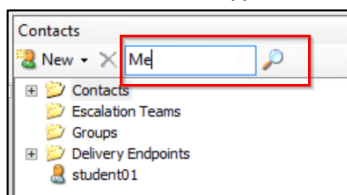
You can configure a PI Notification to receive an email with a hyperlink to a PI Vision display to further diagnose the problem.

Alternately, you can open the **Yeast Realtime PCA** display in PI Vision – use the appropriate bookmark in Google Chrome.

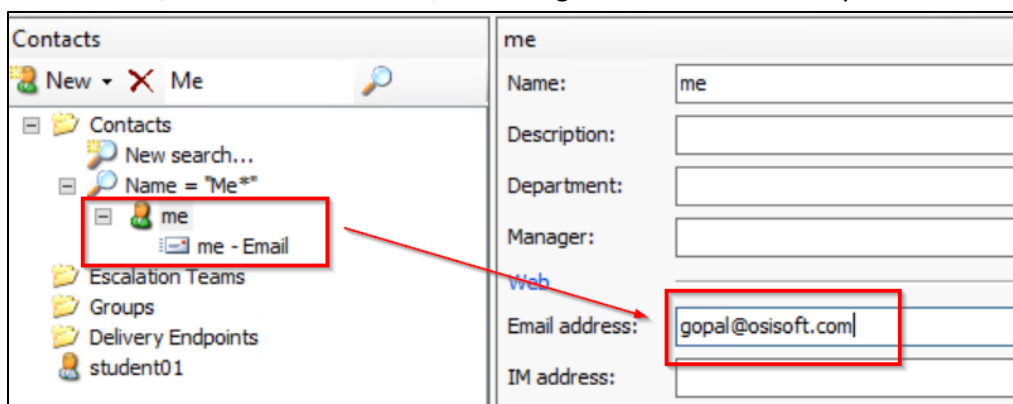


Configure PI Notifications to receive an email (optional)

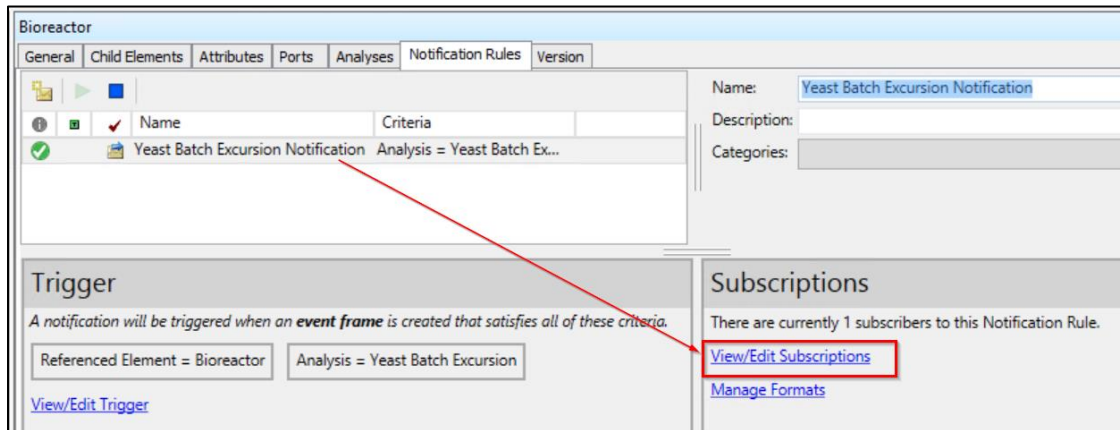
1. In PI System Explorer, navigate to Contacts tab: 
2. In the Search box, type **Me** and click on the  icon to search



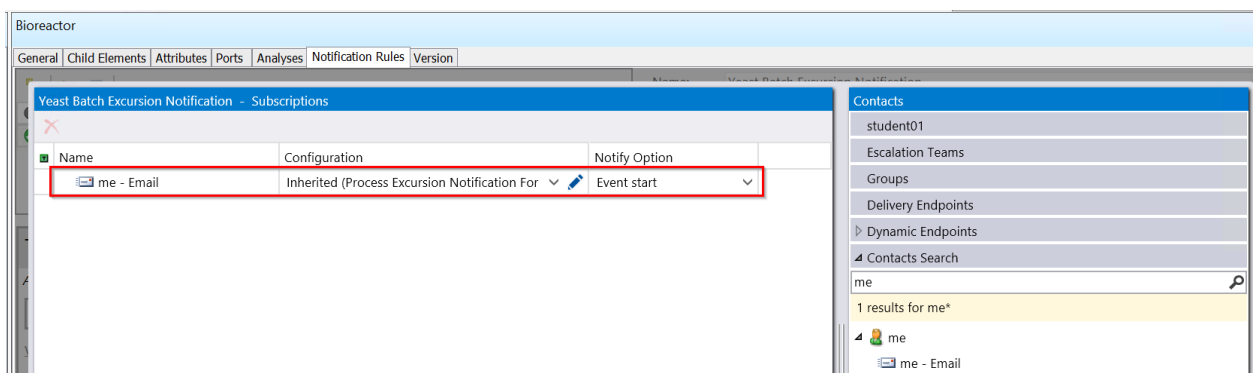
3. In the results, select the contact **Me**, and change the email address to your own:



4. You can verify that you are subscribed to the notification as follows:
  - a. In the **Elements** tab, select the **Bioreactor** element and go under **Notification Rules**
  - b. Select **Yeast Batch Excursion Notification** and click the [View/Edit Subscriptions](#) link

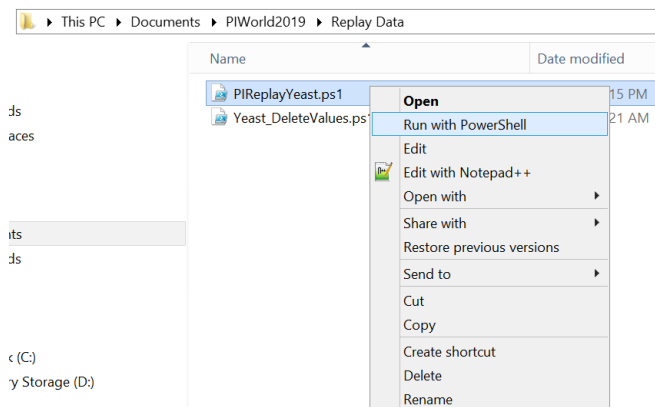


- c. Verify that the contact you just modified (Me) is in the subscribers list:



## Replay the data for Batch U3054

1. Right Click **PIReplayYeast.ps1** in <Replay Data> folder to bring up the context menu, and select "Run with PowerShell"



If you receive a Warning message regarding Execution Policy etc., say “Y” to continue.

2. The script will initialize variables and prepopulate the process limits.

```
Administrator: Windows PowerShell

Initializing variables ...
Getting Source values ...
Populating Limits ...
09-Apr-19 10:20:00 AM
Current Batch Timestep: 0
09-Apr-19 10:30:00 AM
Current Batch Timestep: 1
09-Apr-19 10:40:00 AM
Current Batch Timestep: 2
09-Apr-19 10:50:00 AM
Current Batch Timestep: 3
09-Apr-19 11:00:00 AM
Current Batch Timestep: 4
09-Apr-19 11:10:00 AM
Current Batch Timestep: 5
09-Apr-19 11:20:00 AM
Current Batch Timestep: 6
09-Apr-19 11:30:00 AM
Current Batch Timestep: 7
09-Apr-19 11:40:00 AM
Current Batch Timestep: 8
09-Apr-19 11:50:00 AM
Current Batch Timestep: 9
09-Apr-19 12:00:00 PM
Current Batch Timestep: 10
09-Apr-19 12:10:00 PM
Current Batch Timestep: 11
...
Current Batch Timestep: 77
09-Apr-19 11:20:00 PM
Current Batch Timestep: 78
09-Apr-19 11:30:00 PM
Current Batch Timestep: 79
09-Apr-19 11:40:00 PM
Current Batch Timestep: 80
09-Apr-19 11:50:00 PM
Current Batch Timestep: 81
10-Apr-19 12:00:00 AM
Current Batch Timestep: 82
10-Apr-19 12:10:00 AM
Current Batch Timestep: 0
10-Apr-19 12:20:00 AM
Current Batch Timestep: 0
Process Values: Ready to write Chunk #1: 35 values out of the 85 remaining... Hit any key to continue
```

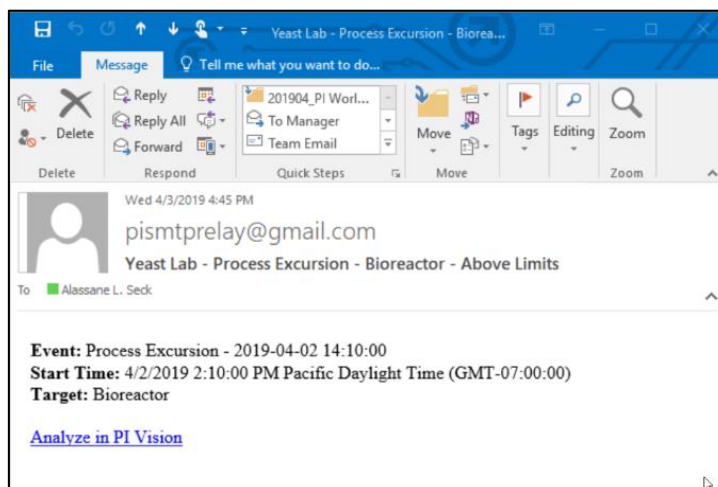
Once it reaches the step shown, it is ready to fill the real-time process values. Hit any key to fill the first chunk of values.

After the first several values of each process variable are written, the script will pause.

```
Ethanol: 3.23302
Level: 46.9313
NH3: 212.187
pH: 5.16068
Temp: 30.2346
Batch: U3054
Batch Active: 1
09-Apr-19 03:50:00 PM
Air: 6510.931
Molasses: 2967.291
Ethanol: 3.42383
Level: 47.20824
NH3: 213.2048
pH: 5.14656
Temp: 30.23326
Batch: U3054
Batch Active: 1
09-Apr-19 04:00:00 PM
Air: 6515.994
Molasses: 2967.255
Ethanol: 3.58691
Level: 47.4661
NH3: 212.4512
pH: 5.1346
Temp: 30.25068
Batch: U3054
Batch Active: 1
Backfilling PCA Analysis and checking for excursions...
6ab9ddb5-d80f-49b6-9da0-d6018ec74283
Process Values: Ready to write Chunk #2: 35 values out of the 50 remaining... Hit any key to continue
```

If you configured PI Notifications to send you an email, you should receive one at this point.

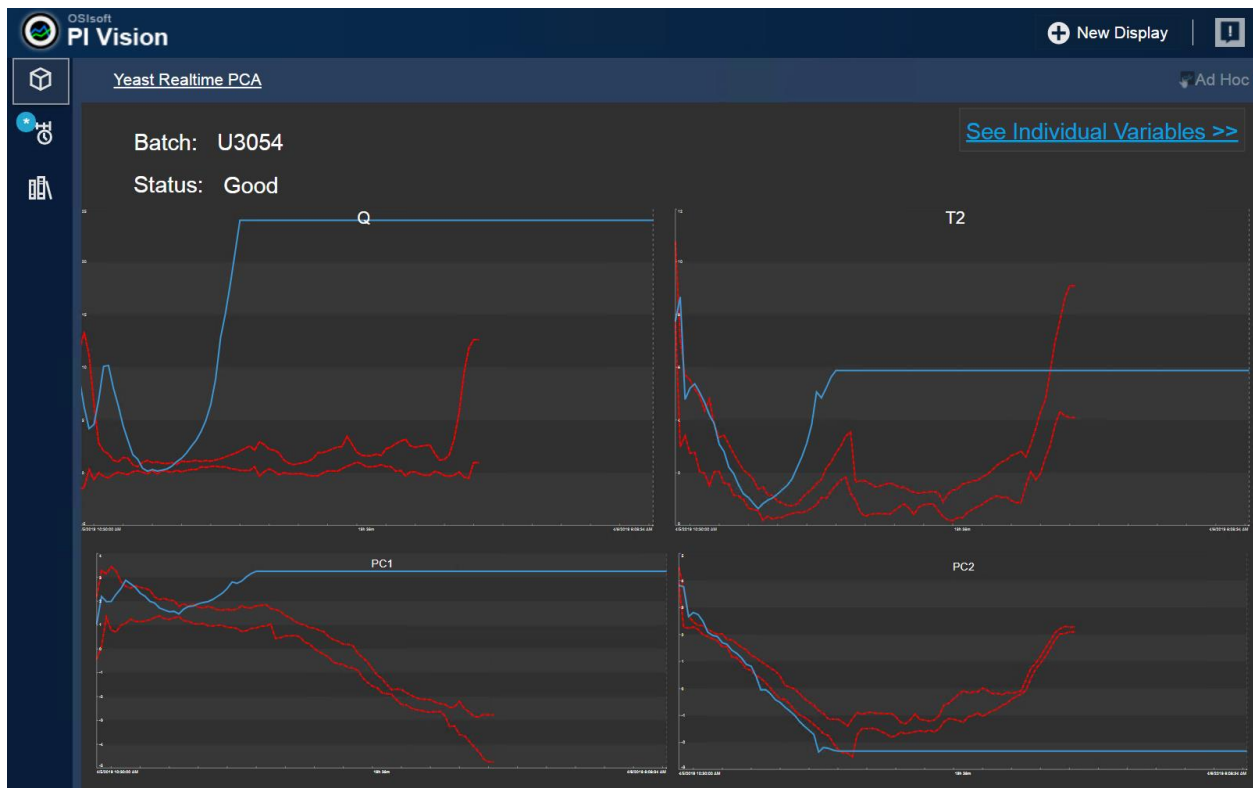
Note that the PI Notification alerts have been configured against T2 and Q limits and not against the individual process variables.



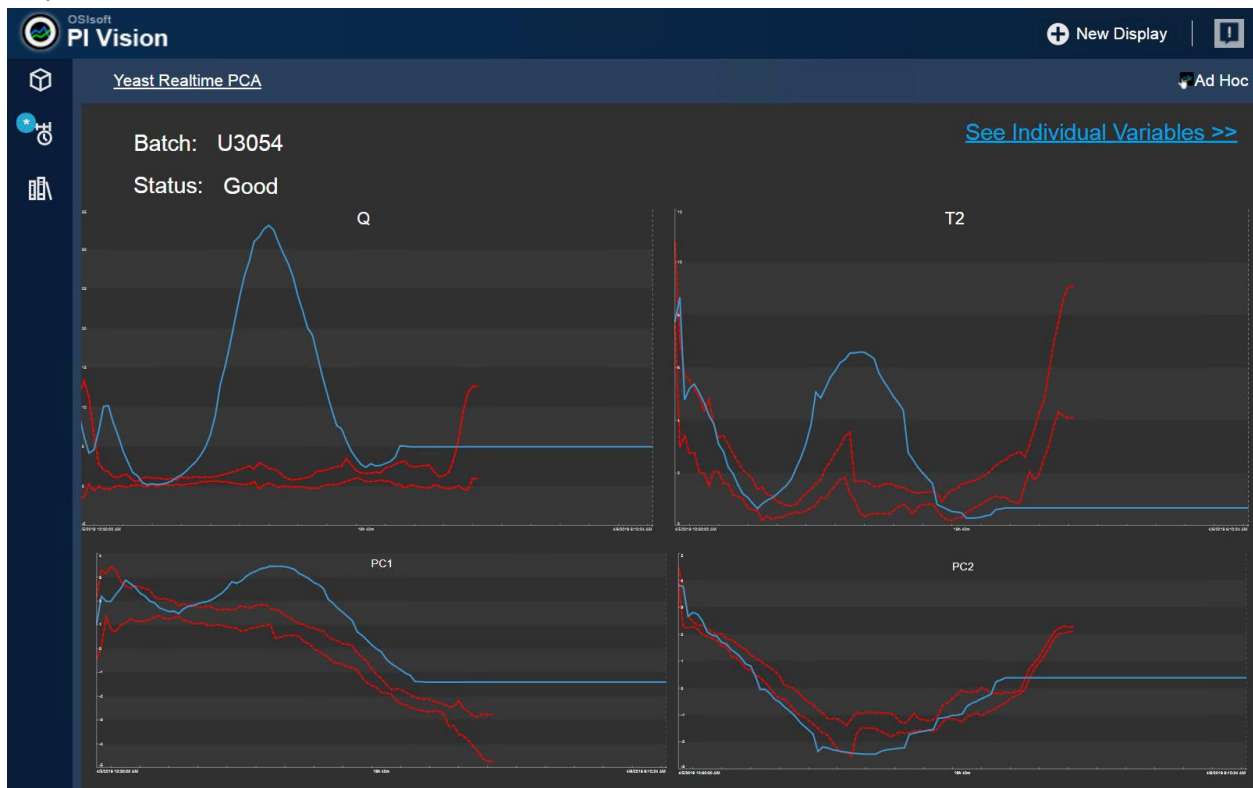
You can also directly navigate to the **Yeast Realtime PCA** display in PI Vision and observe the evolution of the PCA variables.

The latter should clearly show that your process went out of control.

You can navigate to the display showing individual variables to assess which variable went out of limits exactly. For this batch run, it is clear the ethanol exceeded acceptable limits.



3. Play the second chunk of data where the ethanol back under control limits.



## Part III – Model Development Using R – Full Batch Assessment

### Exercise 2 Full Batch Assessment

In this exercise, we prepare the data with time in columns instead of rows for full batch assessment.

See Yeast.html for R script and output.

## Part IV – Model Development Using R – Predict Quality

### Exercise 3 Predict Quality

In this exercise, we use the data format from Exercise 2 but with PLS to predict quality.

See Yeast.html for R script and output.

## Reference Materials

<https://cran.r-project.org/>

<https://shiny.rstudio.com/>

<http://stackoverflow.com/questions/22309236/options-for-deploying-r-models-in-production>

Yeast dataset: <https://landing.umetrics.com/downloads-other-downloads>





Have an idea how to  
improve our products?  
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