Enzyme Reactor Bonsai Brain

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1.0 Introduction

A continuous enzyme reactor simulation has been built with VP Link simulation tool. The goal of the continuous reactor is to avoid the time-consuming operations of the batch reactor including de-inventory, charging, and sterilization.

This model connects to a Bonsai brain that demonstrates the capability of Bonsai to control a complex system such as this in a variety of transient and steady conditions and provide examples of Multi-Concept brain designs.

Use this document and the supplied samples to get started with this problem and learn more about the model and Bonsai!

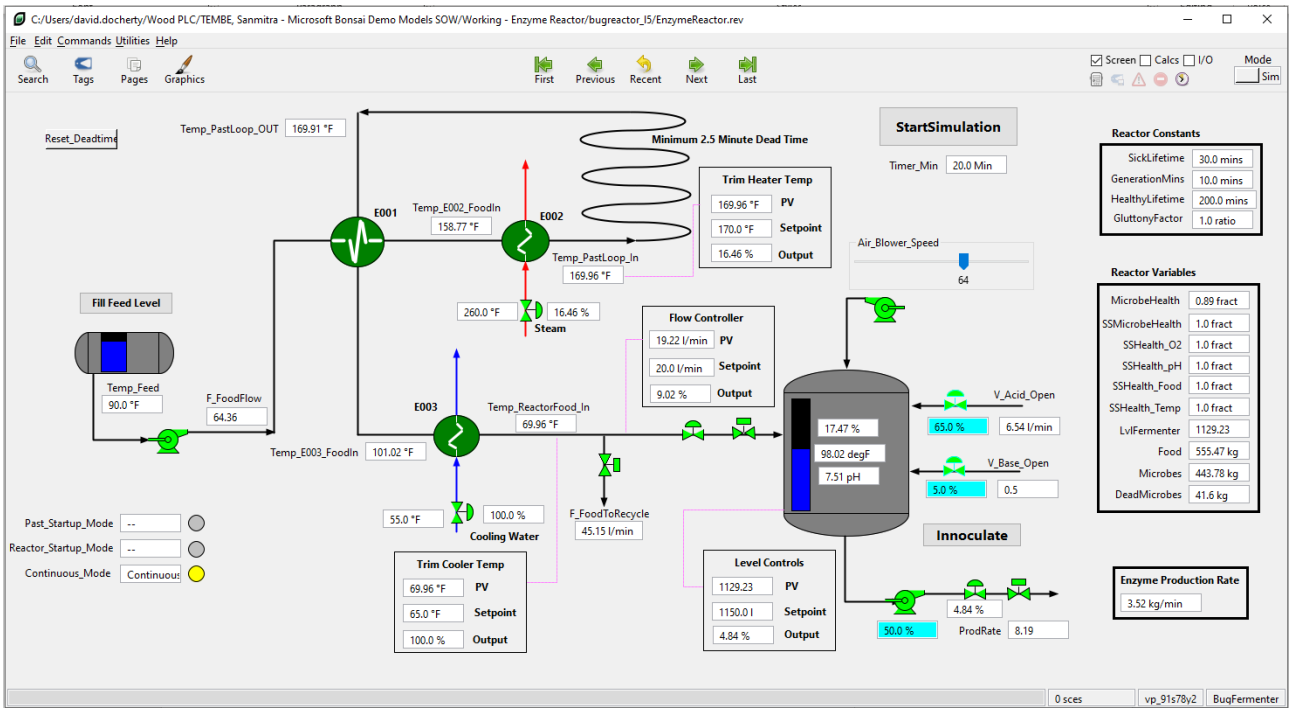


Figure 1-1: Enzyme Reactor Schematic

2.0 Process Description and Control Strategy

In this process, the 'food' for the enzyme producing microbes, with a pH of 7, is pasteurized continuously at 170 F for at least 3 minutes, or 175 F for 2.5 minutes before being fed to the reactor. This is achieved by pre-heating the food in heat exchangers E001 and E002. If the pasteurization criteria are not met, then invasive microbes from the outside world will be introduced into the reactor and wipe out the laboratory microbes which are unprepared to compete with microbes that have adapted to live in the competitive life environment. If the food is heated above 190 F, then the food will start to caramelize on the surface of the steam exchanger, causing it to foul and lose the nutrition required by the enzymes to multiply. If the food has not been pasteurized, it can be diverted to the drain to avoid introducing it in the reactor.

The process starts with the reactor that has been filled with sterilized media including some concentration of feed. Enzyme producing microbes are introduced into the reactor which start to consume the food and multiply. The quantity of enzymes in the reactor grows at an exponential rate, as the rate at which new enzyme producing microbes appear is proportional to the number of those microbes in the reactor.

Enzyme producing microbes grow at the maximum rate at a temperature of 98 F, 17.5% dissolved Oxygen content and pH of 7.5 if there is sufficient feed in the reactor. An excess of food does not make the microbes grow even faster, as there is some limit as to their metabolism. But a scarcity of food does reduce the growth rate and causes some microbes to die, meaning they will never reproduce again, even if the food supply is restored.

The food to the reactor will be automatically diverted back to the feed tank if the flow rate to the reactor falls below 15 l/min. This prevents a low flow situation in the steam heater. This also helps in start-up of the process.

The recycle valve will automatically close when the flow to the reactor is above 25 l/min, as the pump does not need waste capacity flowing back to the food tank at rates above that threshold. There are some flow disturbances associated with the recycle valve opening and closing, but the feed flow controller will restore the flow to the desired setpoint.

The optimum residence time for the reactor is dependent on the growth rate of the enzyme producing microbes in the reactor. If the feed rate to too fast and the residence time is too short, then the microbes can be flushed out of the reactor before they have time to multiply. If the residence time is too long, then the microbes will be starved for food and their growth rate will be lower than the optimum. Ideally, the steady state is such that the production rate out the bottom of the reactor is such that microbes are removed from the reactor as fast as they are growing.

The microbes produce heat when they grow, so the reactor must be cooled to maintain a steady temperature.

The waste product of growing microbes is basic, and as the growth rate increases, acid is required to maintain the pH at the proper level. Manual valves to regulate flow of an acid and a base are connected to the reactor.

The challenge in this case is to control both the temperature and the concentration in the reactor to optimal levels. The problem is particularly hard during start-up as the temperature control needs to be rapid without being overly aggressive to kill off the enzyme producing microbes.

There are effectively 3 'modes' the system can be in. Pasteurisation startup, Reactor startup and Continuous mode. During Pasteurisation startup the system is on full recycle and the focus is getting the loop up to temperature without getting too hot. Once the loop is hot the Reactor is inoculated and feed introduced to it,

the fermentation begins. Initially during this phase the reactor operates without any outflow to build up sufficient Microbe population to move to continuous mode. Once in continuous mode the aim is continuous enzyme production from the reactor outflow.

The following broad aims form the high level control strategy:

- **Maximise Enzyme production:** The overall aim of this process is to produce enzymes, as such the top level goal is to maximise this production. This can be subdivided into two main aims.
    - **Control Reactor Conditions:** Maintain the pH, dissolved oxygen content, level and Temperature in the reactor to maximise growth and production rate of the enzyme producing microbes
    - **Control Feed Conditions:** Ensure the feed into the reactor is at the correct temperature during steady and transient conditions

3.0 State Space

Below are the State and Actions tags that would be defined in the Bonsai Brain. In most cases it can be seen that Bonsai will act upon the setpoint rather than the valve itself. Where that is the case PID loops exist in the model to function as the PID controller.

Table 3-1: State and Action Tags

State Tags	Action Tags
• Enzyme Production Rate (Enzyme_Prod_Rate) • Reactor Level (LvlFermenter) • Continuous Mode status (Continuous_Mode) • Pasteurisation Startup Mode status (Past_Startup_Mode) • Reactor Startup Mode status (Reactor_Startup_Mode) • Button to engage continuous mode (Continuous_Mode_Button) • Button to engage Pasteurisation Startup mode (Past_Startup_Mode_Button) • Button to engage Reactor Starup Mode (Reactor_Startup_Mode_Button) • Total amount of Microbes in the reactor (Microbes) • Total amount of food in the reactor (Food) • Reactor Dissolved Oxygen % (Reactor_O2) • Reactor temperature (Reactor_Temp) • Reactor pH (Reactor_pH) • Temperature of food inlet to Steam Heater (Temp_E002_FoodIn) • Temperature of food feed (Temp_E003_FoodIn) • Temperature into Pasteurisation loop (Temp_PastLoop_In) • Temperature out of Pastuerisation loop (Temp_PastLoop_OUT) Temperature of feed into reactor (Temp_ReactorFood_In)	• Acid Valve (V_Acid_Open_Vlv) • Base Valve (V_Base_Open_Vlv) • Setpoint of Reactor Level Controller When in Reactor Startup Mode (Reactor_Level_Setpoint_St) • Setpoint of Reactor Level Controller When in Continuous Mode (Reactor_Level_Setpoint_C) • Setpoint of Feed Flow Controller When in Reactor Startup Mode (FlowSetPoint_St) • Setpoint of Feed Flow Controller When in Continuous Mode (FlowSetPoint_C) • Setpoint of Trim Cooler Temperature Controller (ReactorFoodInlet_PastLoop_TempSetpoint) • Setpoint of Steam Heater Temperature Controller (PastLoop_TempSetpoint) • Air flow into reactor (Air_Blower-Speed)

4.0 Model Description

The enzyme reactor uses a number of different calculations that allow the liquid flow, heat transfer and reactor action to occur. The following sections describe the model and modelling process in detail.

4.1 Liquid Flow Network

Liquid flow is modelled in VP Link using a liquid flow network tool. This tool creates a matrix of pressure nodes and flows between the nodes that is solved dynamically at every timestep. The liquid flow in this model is the 'food' for the microbes in the reactor.

The tags that execute the Liquid Flow Network are built by a tool called LFNGEN. The input file that describes the network is an Excel sheet. A Liquid Flow network is made up of pressure nodes and flow links between those nodes. Pressure nodes have no liquid holdup and have a design pressure. Flow links connect two pressure nodes and represent a design flow rate between the two pressure nodes. These flow links essentially provide a resistance to flow and may or may not have a variable resistance (=control valve) in the line. Flow links can have block valves in the line that completely block the flow. In the Excel sheet, the user specifies pressure nodes and flow links between those nodes. In addition, a tank can be specified that acts like a pressure node.

The Pressure Nodes are endpoints for the Flow Links. They have a design pressure as well. Normally the pressure in these pressure nodes will vary during the course of the simulation as flows increase and decrease. But the pressure of the atmosphere is a constant for this simulation. The Flow Tags are typically pipes with zero or more control valves and block valves. If there is a control valve in the line, it is specified in the Valve Tag column.

The liquid flow network tags are modelled following design parameters: the feed pump can pump out a maximum of 98 l/min of 'food' for enzyme producing microbes in the reactor. This flow is regulated by feed flow control valve "V_React". The feed is pasteurized in a trim heater with steam coming in at 260 F. The steam flow is throttled by temperature control valve "HeatIn" to maintain the required pasteurization temperature. The pasteurized feed is cooled in trim cooler with cooling water coming in at 55 F. The cooling water flow is throttled by cooling water valve "CWPID" to maintain the required reactor inlet temperature (the required inlet temperature will vary depending on the reactor state and is something the Bonsai brain will have to decide). The acid and the base flows to the reactor to maintain the desired pH level in the reactor are throttled by "V_Acid_Flow" and "V_Base_Flow". The product from the reactor is pumped under level control through level control valve "V_Sepr". The food to the reactor will be automatically diverted back to the feed tank through block valve "V_Recycle_Open", if the flow rate to the reactor falls below 15 l/min. The recycle valve will automatically close when the flow to the reactor is above 25 l/min, as the pump does not need waste capacity flowing back to the food tank at rates above that threshold. The dissolved oxygen concentration in the reactor required for the aerobic reaction is maintained by the air blower speed.

4.2 Heat Transfer

The liquid food feed is maintained at 90°F before passing through a heat recovery heat exchanger and being heated by the outlet of the pasteurisation loop. It then passes through the steam heater which is intended to heat the food above the pasteurisation temperature of 170°F-175°F. The food passes through the heat recovery heat exchanger which cools it down before going through a cooler to reduce the temperature to the correct setpoint for the reactor.

Inside the reactor temperature is impacted by the following variables- Microbial respiration (adds heat), Inlet flow of fluids at different temperatures to reactor mix and addition of oxygen via the air blower (cools the reactor down).

The calculations for the countercurrent heat exchangers require solving two simultaneous equations governing the heat transfer between streams. The Heat exchanger Calcblock solves the two equations that govern a heat exchanger simultaneously, the overall heat balance and the heat transfer equation:

$$Q = (dm/dt) * Cp * DT.$$

Where **Q** = Heat, **Cp**= Heat capacity of fluid, **DT**= temperature change, **dm/dt** = change in mass with time

The calculation assumes that the exchanger is symmetrical, i.e., there is no difference between the shell side and tube side. There is a provision for an extra heat term in case heat in generated inside the exchanger by a reaction. The Calcblock calculates the pseudo steady state values for the exit temperatures. However, these steady state values may optionally be put through a first order lag before appearing as output values of the tag. In this case, small first order lags (of order 0.1 minutes) are introduced for the heat exchangers to introduce some time dependency into the calculations. The inputs to the calculation are the

The outlet of the pasteurisation loop uses the deadtime algorithm. This means a delay of 180 (s) / Flowrate through loop (l\min) before the loop inlet temperature is seen at the outlet, this deadtime adds some complexity to the control problem. At a typical flowrates of 60 l\min this would lead to a residence time in the loop of 3 minutes. The recycle loop ensures that even if the flow into the reactor is low the total flow through the loop will be similar and ensure enough residence time and pasteurisation.

The temperature calculation in the vessel utilises the VP Link Mixtemp algorithm. This factors in the temperatures of the flows into the vessel (feed food rate and acid\base flow) as well as the residual heat of the mass inside the vessel. Additionally a 'heat term' is added to the calculation, this factors in the cooling provided by the air blower and the heat generated by microbial respiration. Each time step a new temperature will be calculated based on a heat balance between the residual heat, added heat and mixing of new fluid into the vessel.

When there is a low number of microbes the temperature is straightforward to control using the food inlet temperature, however as the number of microbes increases the additional heat they generate will lead to a too high temperature (above 105°F) if action is not taken. If too many microbes are present it is possible that they will overproduce heat such that it is difficult to maintain the temperature and Microbes will stop reproducing.

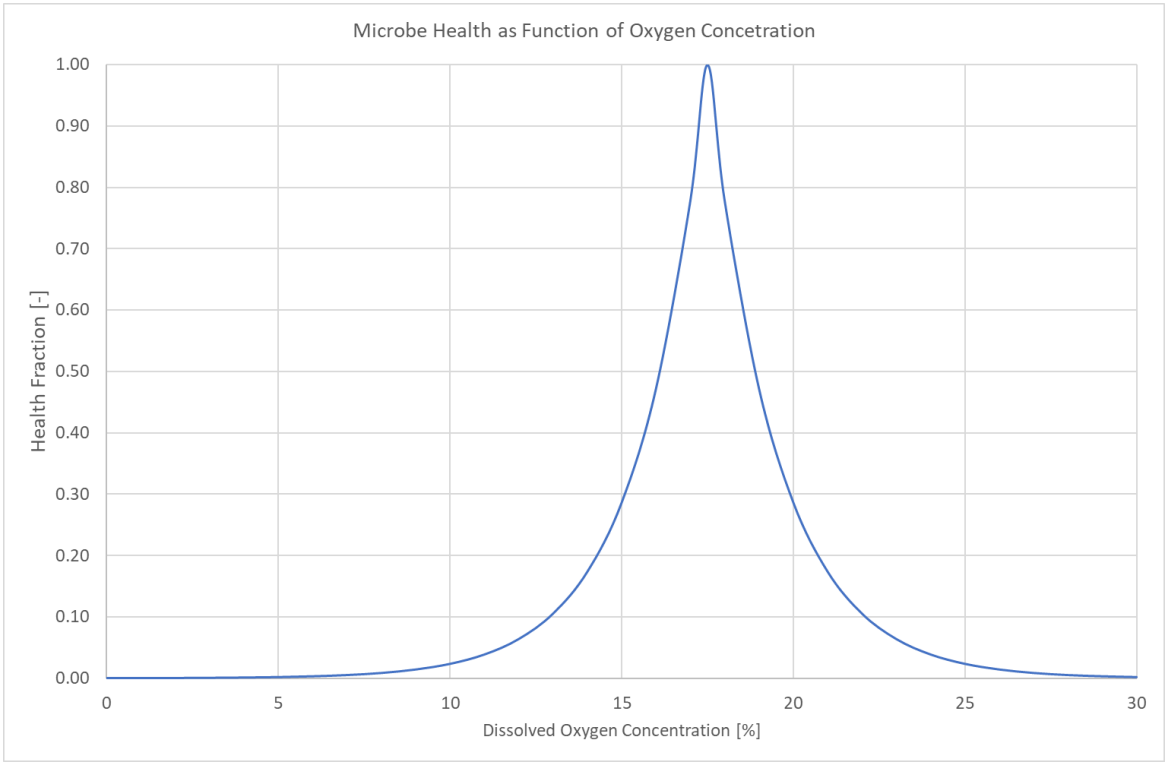
4.3 Microbial growth

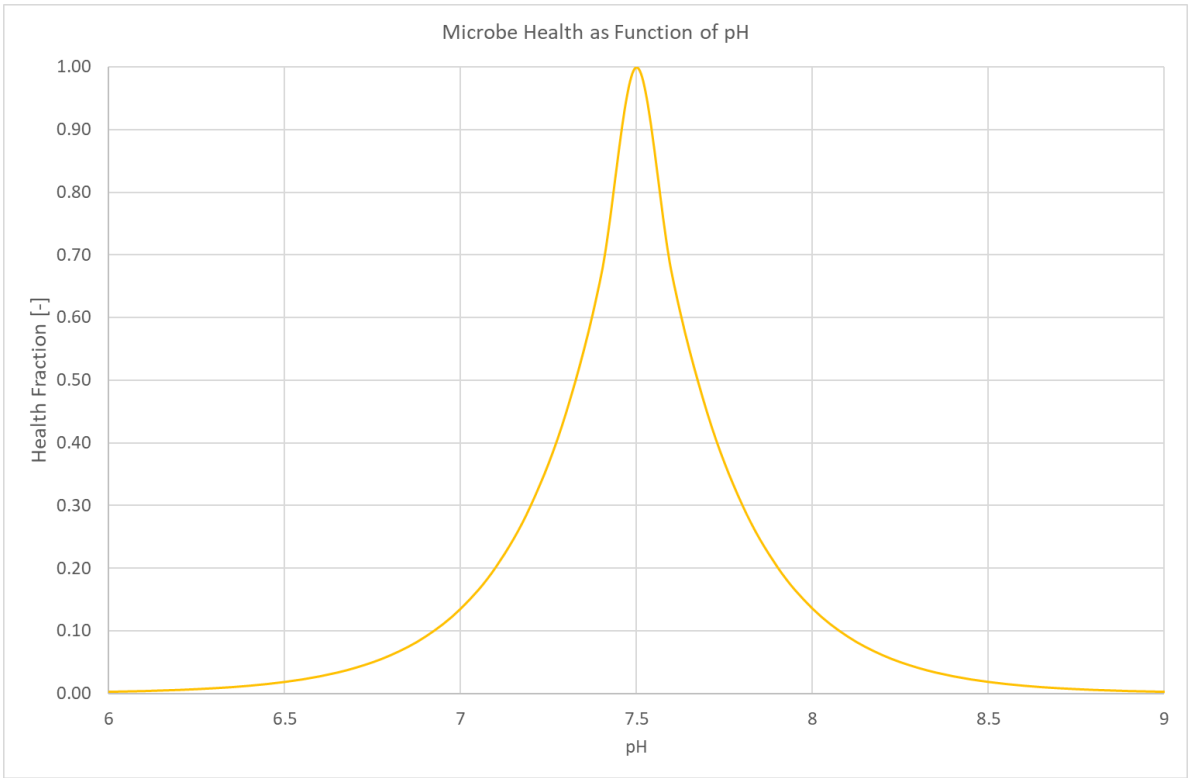
Microbial growth is based upon the following 4 factors:

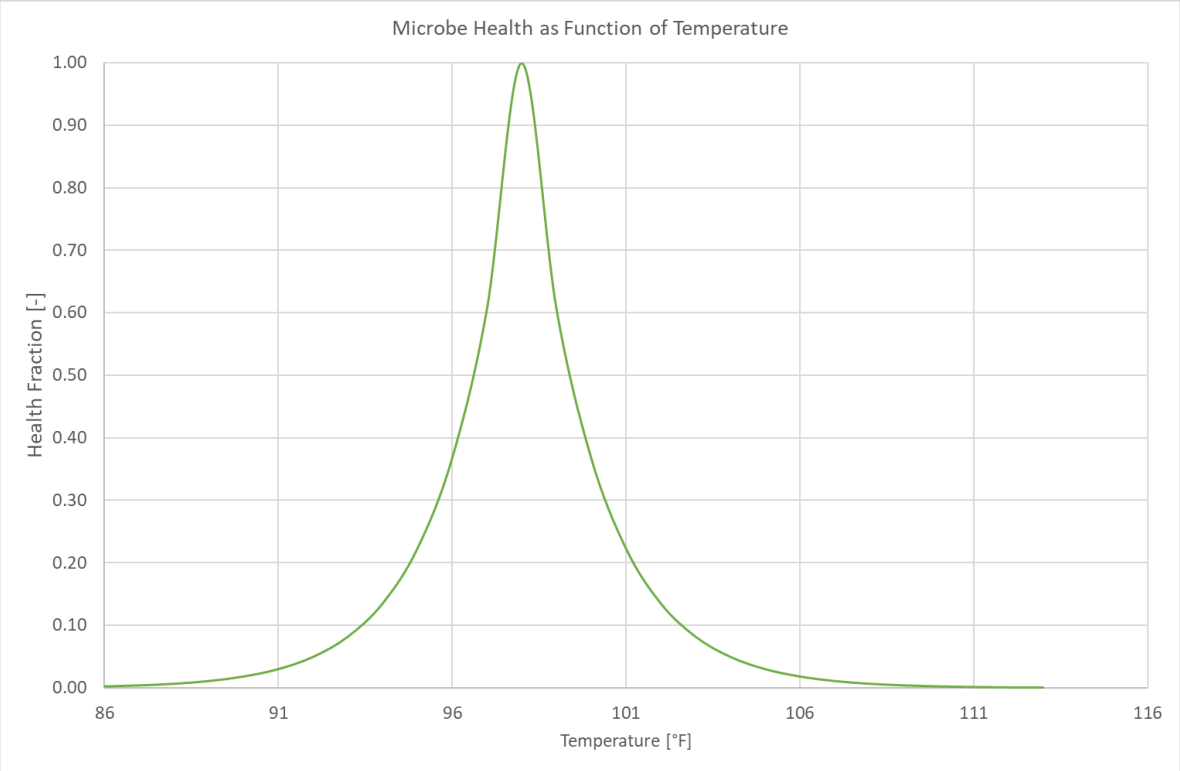
- Availability of Microbe 'food'
- pH inside reactor
- Temperature inside reactor
- Dissolved Oxygen content

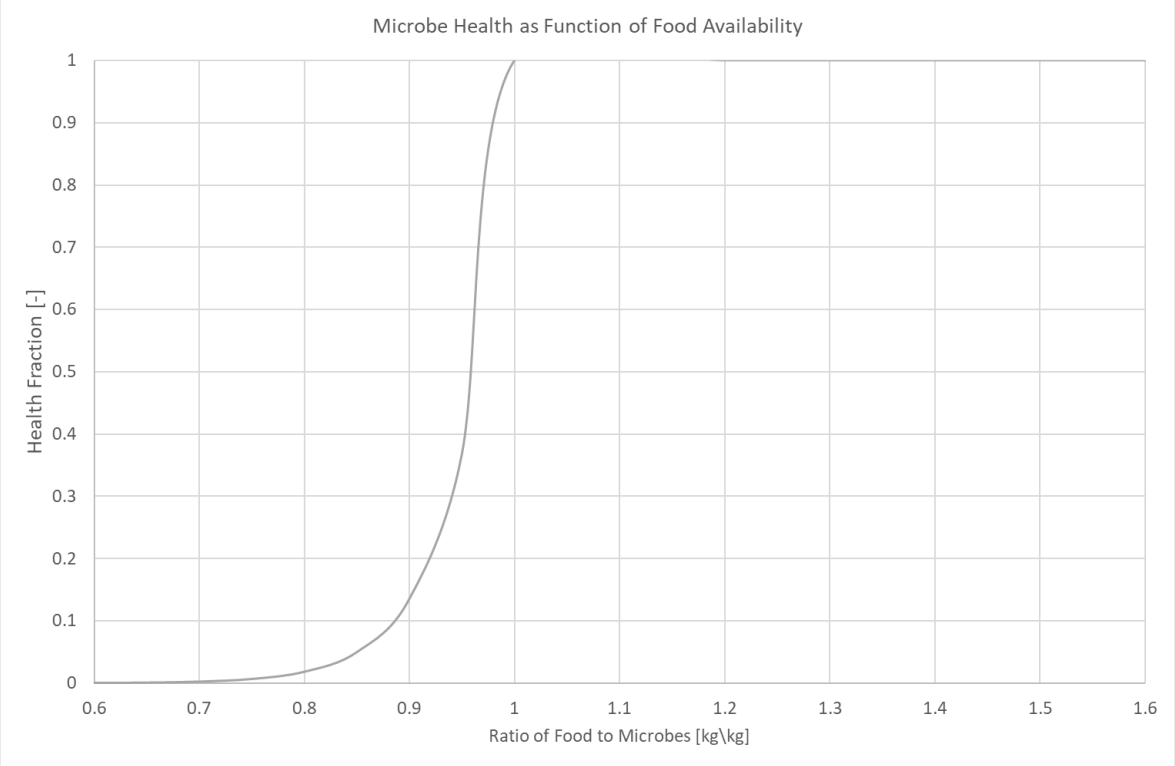
Each factor uses a distribution to determine the 'health' of the microbes based on the variable in question. The

health factors are multiplied by each other to give an overall 'MicrobeHealth' factor. The distributions of the different factors are shown below.









Microbial growth will then occur based on the following formula

(Microbes x MicrobeHealth factor x Constants) / GenerationMinutes

Generation Minutes is a constant that determines how long it takes the healthy Microbes to double (set at 10 minutes). The growth of the microbes will use up available food at ratio determined by the 'GluttonyFactor'- i.e. how much food does 1 kg of microbes use up (set at a ratio of 1). If the health of the Microbes is not equal to 1 then a proportion of them will become 'sick'. Sick microbes will survive for 3 times the generation minutes before dying, whereas healthy microbes will live for 20 times the generation minutes.

A mass balance is performed on the microbes that will calculate the total amount of microbes in the reactor , both for 'alive' and 'dead' Microbes. This balance depends on the growth rate, microbe health and production rate out the bottom of the Reactor. Dead microbes still contain the enzyme and are thus able to contribute to enzyme production but are not able to reproduce, while live microbes will continue reproducing.

The control challenge in the reactor is to maintain the health of the microbes by controlling the various contributing factors and then to produce microbes out the bottom at the same rate they are growing such that a continuous enzyme production is reached.

4.4 System Operating Modes

Three system operating modes are defined:

- Pasteurisation Startup
- Reactor Startup
- Continuous Mode

A calculation exists in the model to determine which mode is active. If the feed pump is on but the reactor inlet valve is closed and the Reactor outlet valve is closed then this is Pasteurisation Startup mode. If the pump is on and the reactor inlet valve open then this is defined as Reactor startup. If the pump is on and both valves are open then this is defined as Continuous mode.

During reactor startup the tank starts at a relatively low level (400 l) and will increase to a level somewhere above 1000 l before switching to continuous mode. Operators know that low flowrates are best initially to encourage microbe growth and as such maximum flow setpoint during this phase should be limited to 20 l\min.

These calculations replicate the function of a supervisory PLC or DCS. Clearly if the feed pump is not running then the system is not operating. Logic and\or operator action would prevent food being added to the reactor without pasteurisation confirmed. Operators know that some microbial growth needs to occur before continuous mode can be activated and as such would not open the bottom valve until they were satisfied.

Different actions for the Flow and level setpoints are specified depending on the mode. In Reactor startup mode operators know that a low flow and a high level setpoint are required in the reactor and thus the action bonsai can take is limited to this range. In continuous mode there is more freedom to determine the optimum level and flow setpoints. The model will use the appropriate setpoint depending on which mode is active.