MELiSSA

TECHNICAL NOTE

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TECHNICAL NOTE TN83.6

System model approach of the liquefying compartment

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APPROVAL

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TABLE OF CONTENT

1. Introduction

The aim of the study is to support EPAS in defining and tuning the level 0 control of the liquefying compartment of the MELiSSA loop.

The selected control functions to be studied are:

- temperature in the bioreactor
- temperature in the influent and filtrate tanks
- liquid volume in the bioreactor
- pH in the bioreactor
- pressure in the gas phase of the bioreactor
- flow rate in the gas analysers

The optimisation and validation of the control are based on tests which can be realised:

- in simulation, which requires development of simplified models including:
  - multi-physics models for the different parts of the pilot (thermal model for temperature, thermo-fluid model for pressure, chemical model for pH …)
  - instrumentation models (sensors and actuators)
  - environment models (disturbances)
  - level 0 control models, derived from the PLC program
- on the pilot, in real operation conditions (meaning with the inoculum), and once the automation and control functions are programmed in the PLC.

The aim of these tests is to check that the systems acts automatically like expected and the control specifications are respected.

Both kinds of tests (in simulation and on the pilot) are to be performed. This report is dedicated to the first kind of tests, and describes the models developed for control evaluation purpose, and the simulation results. The validation of the models is done by comparison between real measures and simulation outputs.

2. System model for bioreactor temperature control

2.1. Pilot requirement

It is necessary to maintain a stable temperature, as fluctuations in temperature can cause a disturbance in the bacteria population.

2.2. Process description

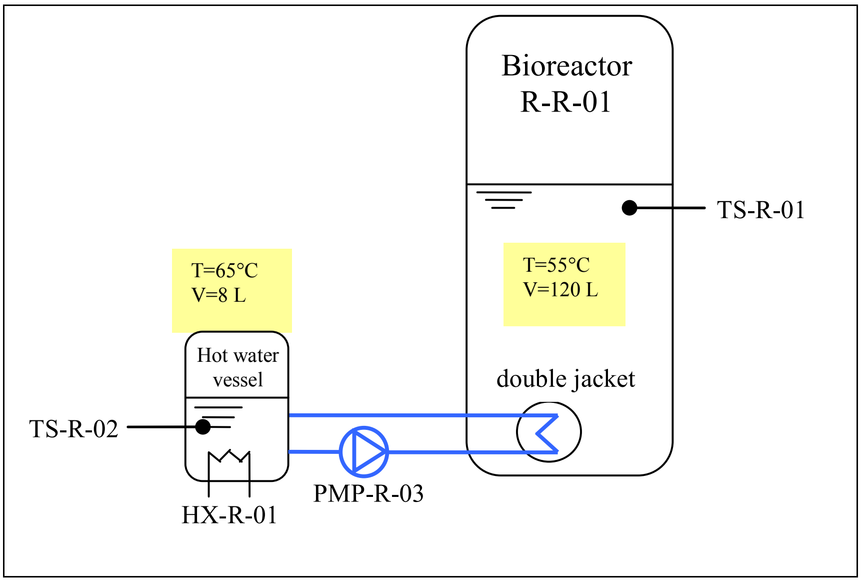


Figure 1: simplified process & instrumentation diagram for temperature control

The temperature is regulated by heat transfer between the reactor content and heating fluid (hot water).

2.2.1.Sensors

- Temperature in the bioreactor: TS-R-01.
- Temperature of the warm water bath: TS-R-02

2.2.2.Actuators and manipulated variables

- Heating via hot fluid (water):
  - The temperature of the hot fluid (≈ 65 °C in steady state condition) is controlled by an electric heater HX-R-01 (maximum power = 2 kW)
  - The hot fluid flow rate is constant (20 L/min for 1.5 metres head)
- No cooling device.

2.2.3.Disturbances

- Temperature of the influent product (≈ 4 °C) which is fed semi-continuously
- Temperature of the recirculation product from filtration
- Thermal losses

- Fluctuation of the ambient temperature

2.2.4. Control

2.2.4.1. *Specification*

- Max constraint = 60 °C
- Steady state set point = 55 ± 0.5°C
- Start-up set point = ramp from 20 to 55 °C (max ramp to be defined)

2.2.4.2. *Control strategy*

- A cascaded loop strategy is implemented in PLC Quantum (concept language):

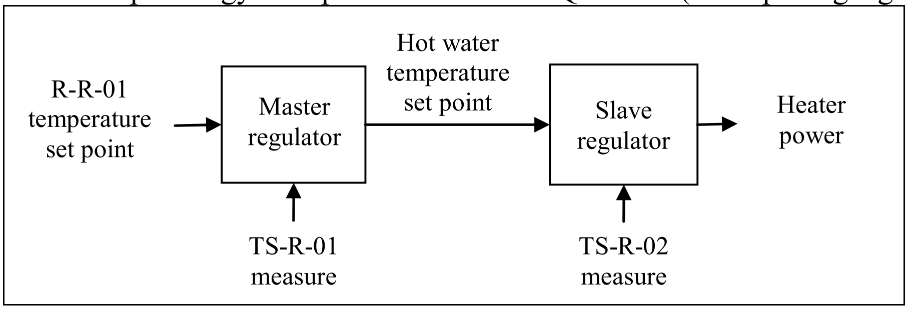


Figure 2: temperature control strategy

- The control period is 1 min for both regulators.
- PI (Proportional Integral) regulators are used.
- The output of the slave regulator is sent to a PWM (Pulse Width Modulator) which steers the heater HX-R-01.

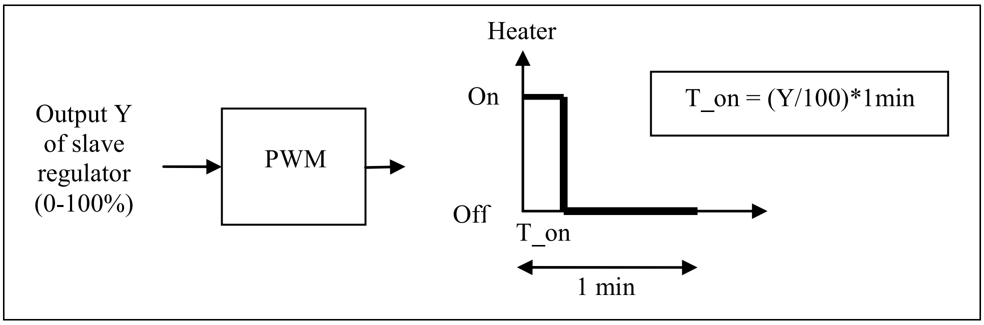


Figure 3: temperature on-off control

2.2.4.3. *PLC code*

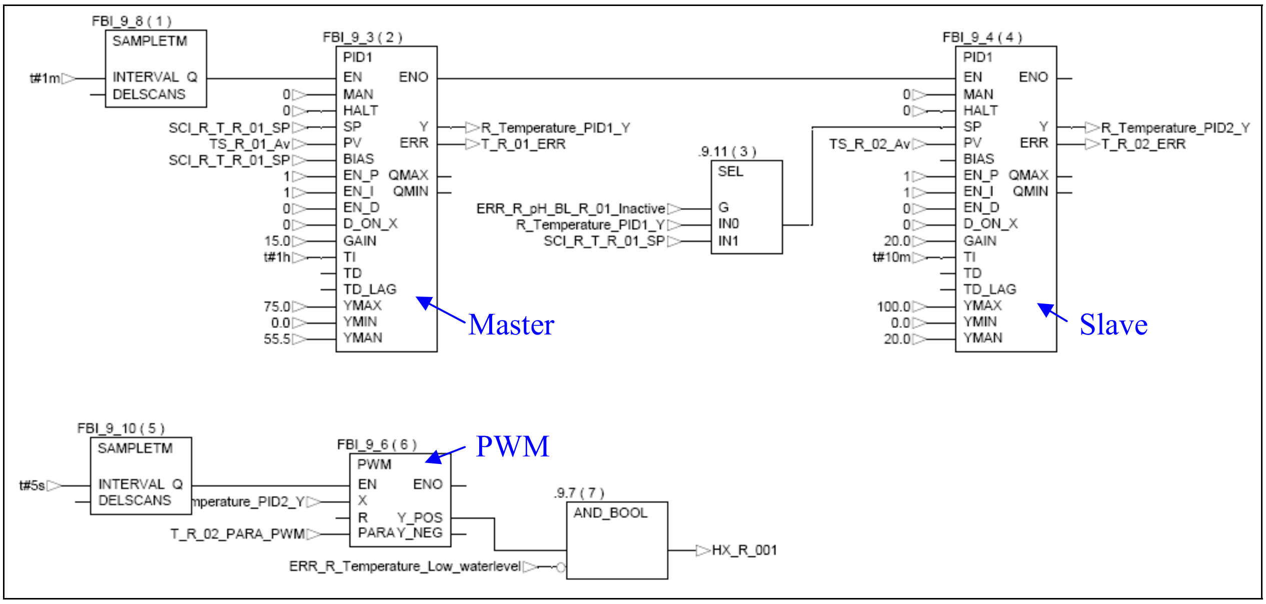


Figure 4: PLC blocks for temperature control

2.3. Model

2.3.1.Structure, equations and parameters

The thermal model of the bioreactor and its environment and control is developed with Simulink.

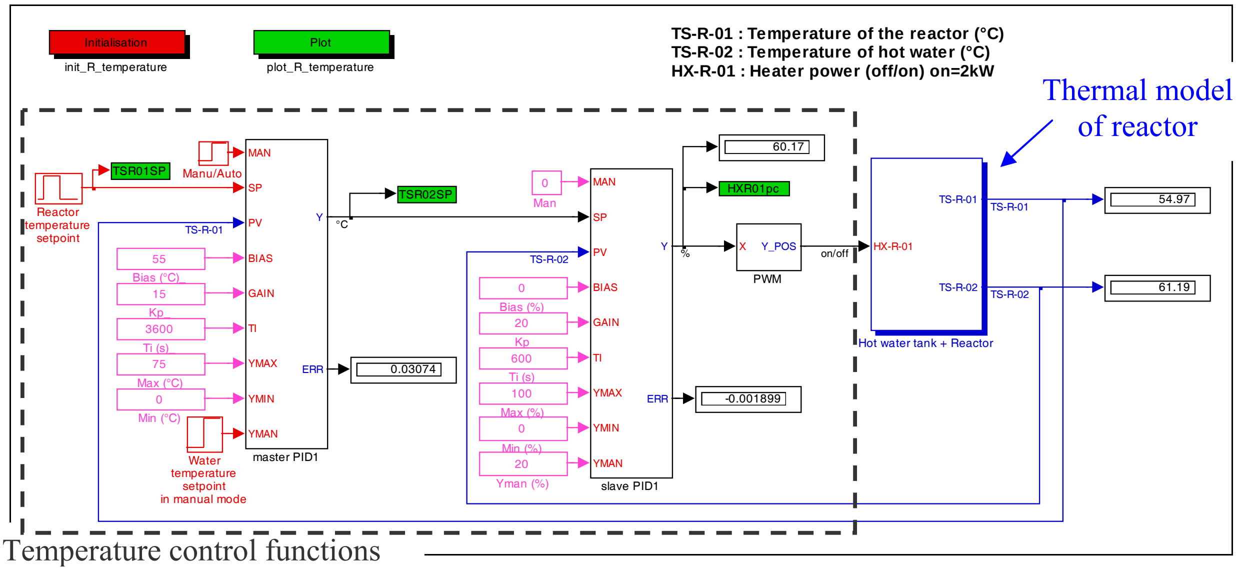


Figure 5: Simulator diagram dedicated to temperature control

The simulator is made up of two parts:

- The first part replicates the control functions which are programmed in the PLC:
  - 2 cascades PID regulators
  - 1 PWM which steers the heater
- The second part models the thermal exchanges between the reactor and the heating fluid:
  - Three thermal capacities of fluid are considered (fluid in the hot water tank, fluid in the double jacket, fluid inside the reactor)
  - One heat capacity is considered (wall between the liquid in the double jacket and the liquid inside the reactor)
  - The considered heat flows are:
    - Heat source to the hot water tank coming from the steering heater
    - Heat transfer between the hot water tank and the fluid in the double jacket due to the circulation of water
    - Forced convection between the double jacket and the wall
    - Free convection between the wall and the fluid inside the reactor
    - Heat flow during influent feeding
    - Various thermal losses with the ambient environment

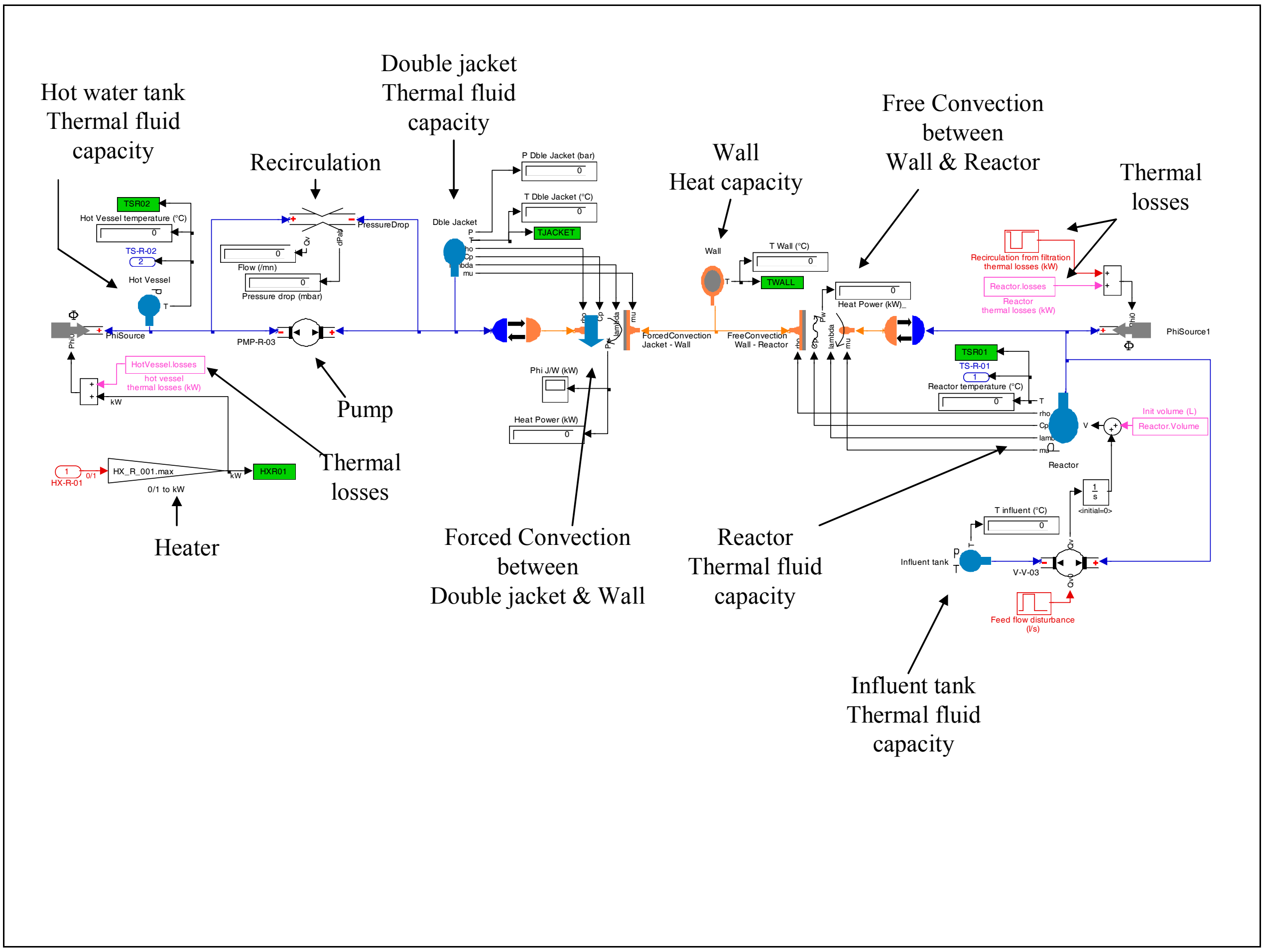


Figure 6: thermo-fluid modelling

The parameters are listed in appendix 8.1.

2.3.2. Validation

2.3.2.1. *Static validation*

In nominal conditions (i.e. with recirculation flow), both simulation results and process measurements give the same operating points (see figures below):

- Reactor temperature = 55 °C
- Hot water temperature ≈ 61.5 °C
- Heater steering ≈ 60 % = 1.2 kW

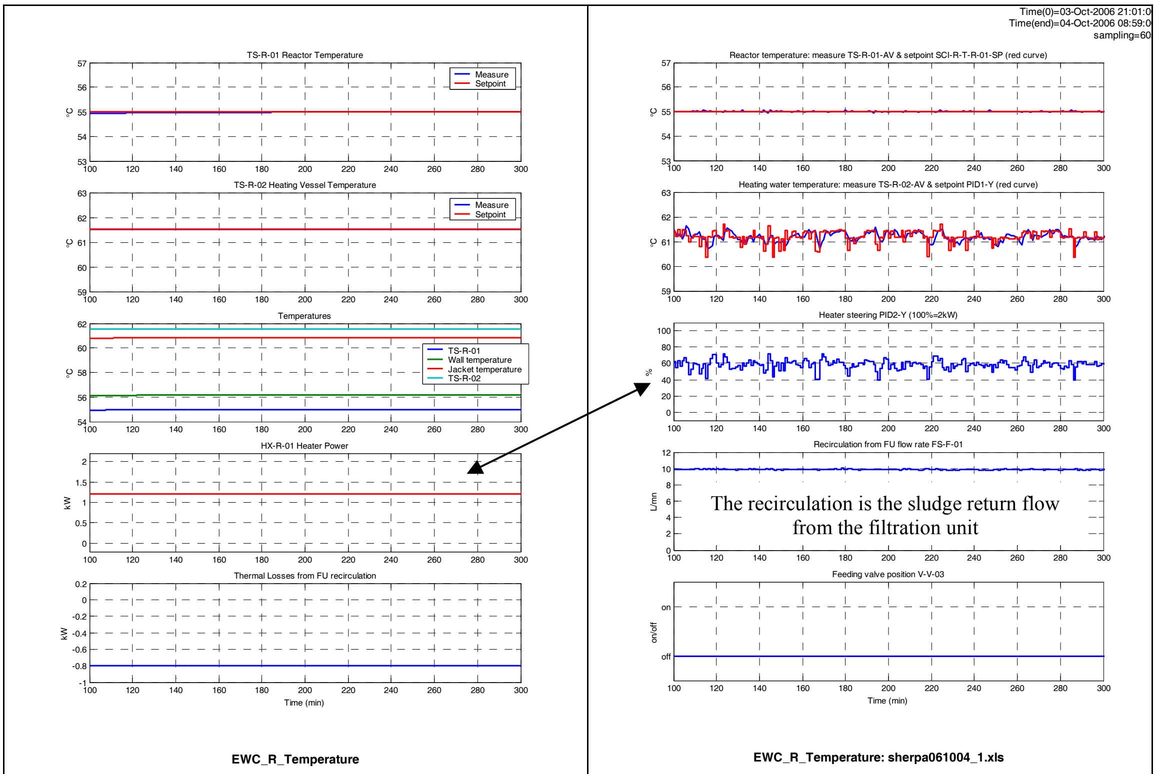


Figure 7: simulation results | **Figure 8: reactor measurements**

Reactor temperature operating points with recirculation ON

With no recirculation flow, both simulation results and process measurements give the same operating points (see figures below):

- Reactor temperature = 55 °C
- Hot water temperature ≈ 56.5 °C
- Heater steering ≈ 20 % = 0.4 kW

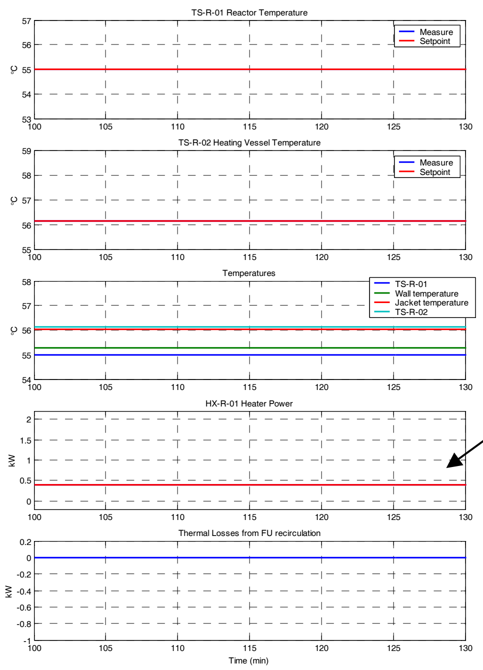


Figure 9: simulation results

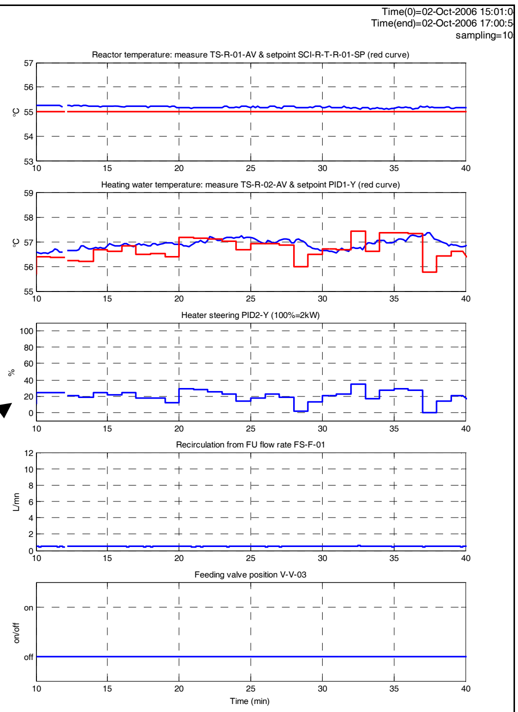
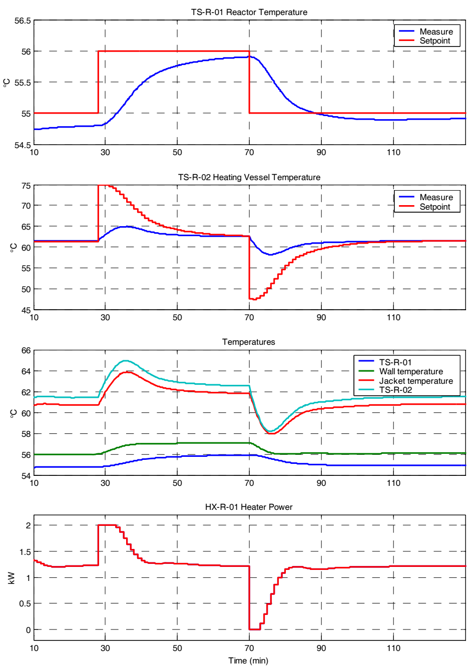


Figure 10: reactor measurements

Reactor temperature operating points with recirculation OFF

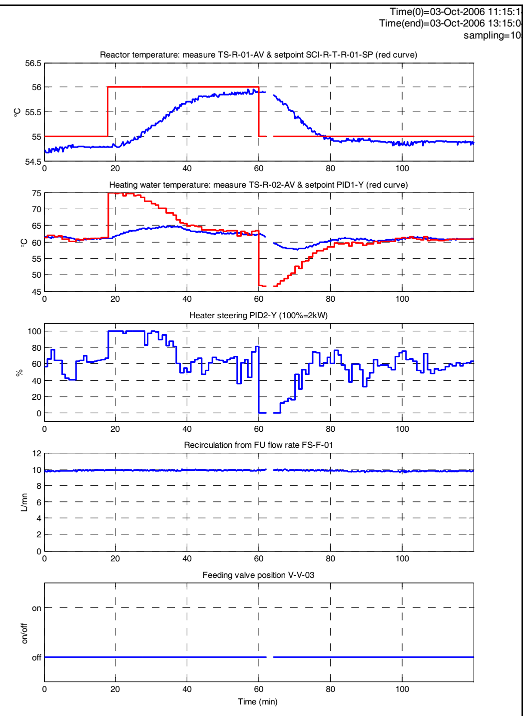
2.3.2.2. *Dynamic validation*

For a set point change of ±1°C, both simulation results and process measurements give similar responses (see figures below):



EWC_R_Temperature

Figure 11: simulation results



EWC_R_Temperature: sherpa061003_2.xls

Figure 12: reactor measurements

Reactor temperature responses to set point changes

2.3.2.3. *Conclusion: predictive capacity of the model*

The responses given by the model are similar to the measured ones. Therefore, regarding temperature control performances, the model is valid to predict the behaviour of the process (the reactor) both to set point changes or disturbances.

2.3.3. Simulation results

2.3.3.1. *Performances related to set-point changes*

The settling time within 95% is around 25 minutes, with a slight overshoot.

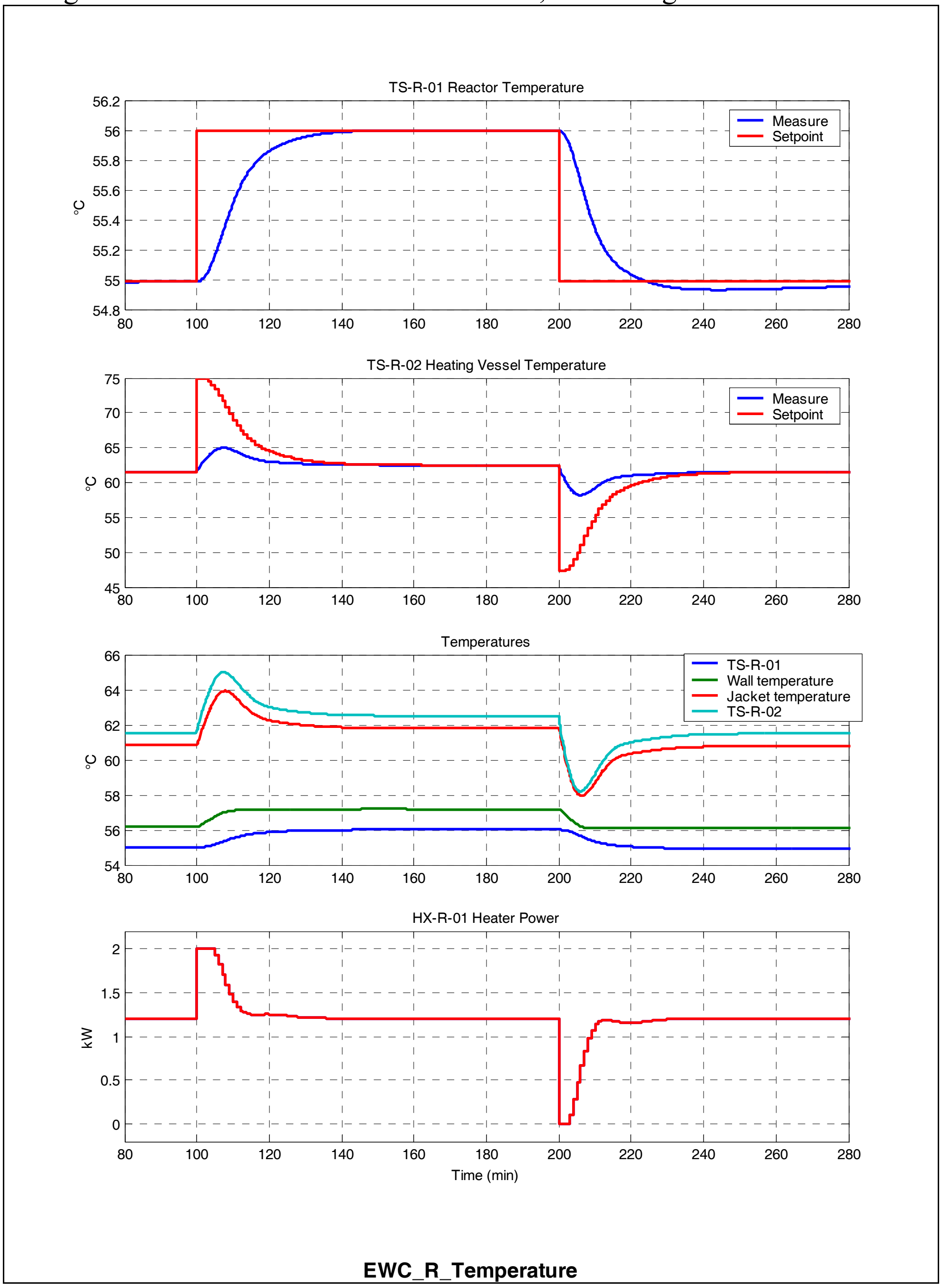


Figure 13: simulation of temperature set-point changes

2.3.3.2. *Performances related to disturbances*

Feeding of 1 litre of product at 10°C makes the reactor temperature decrease by 0.4°C.

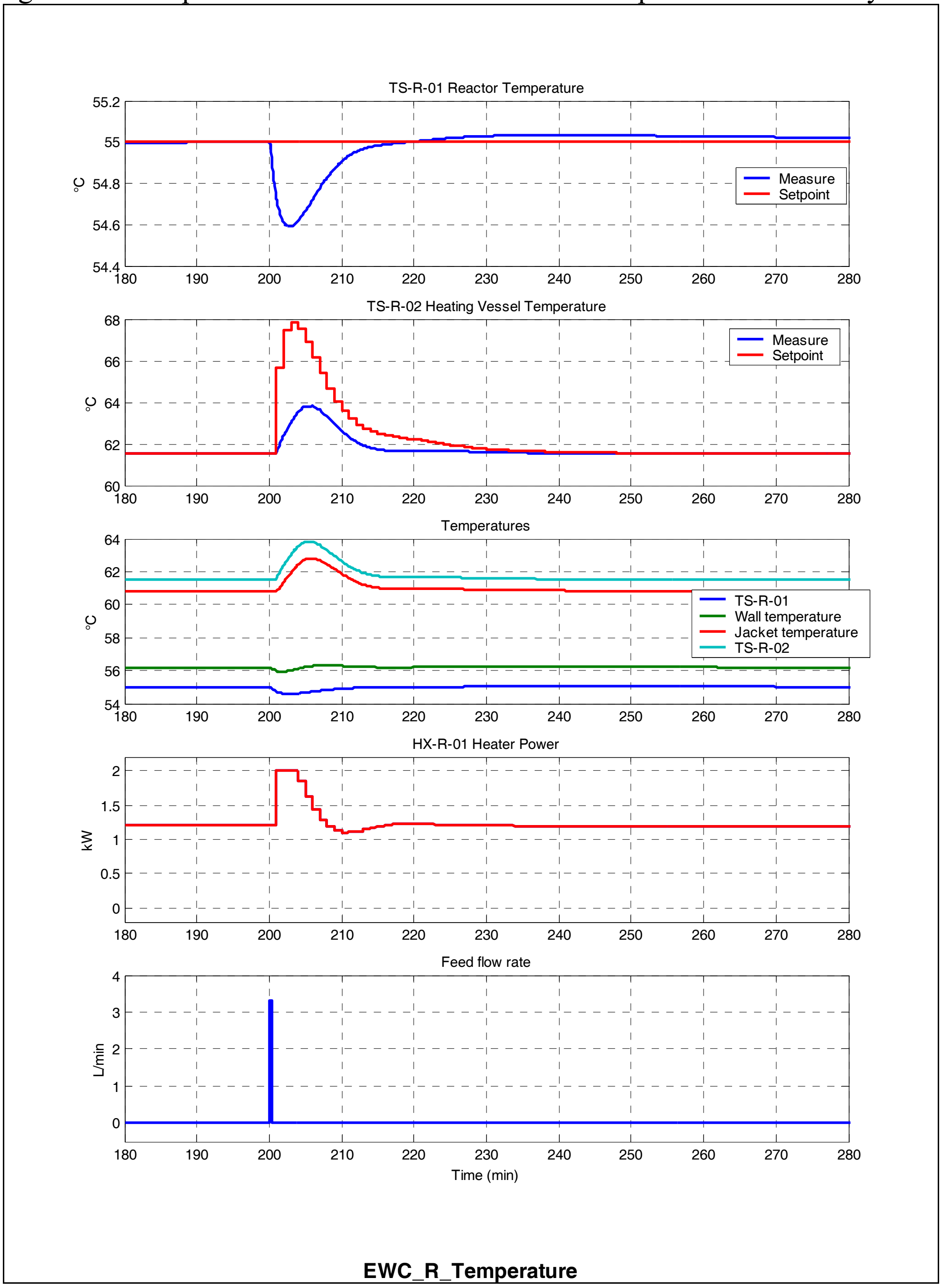


Figure 14: simulation of product feeding (semi-continuous)

A stop or restart of the recirculation from the filtration unit makes a ±0.5°C change in the reactor temperature.

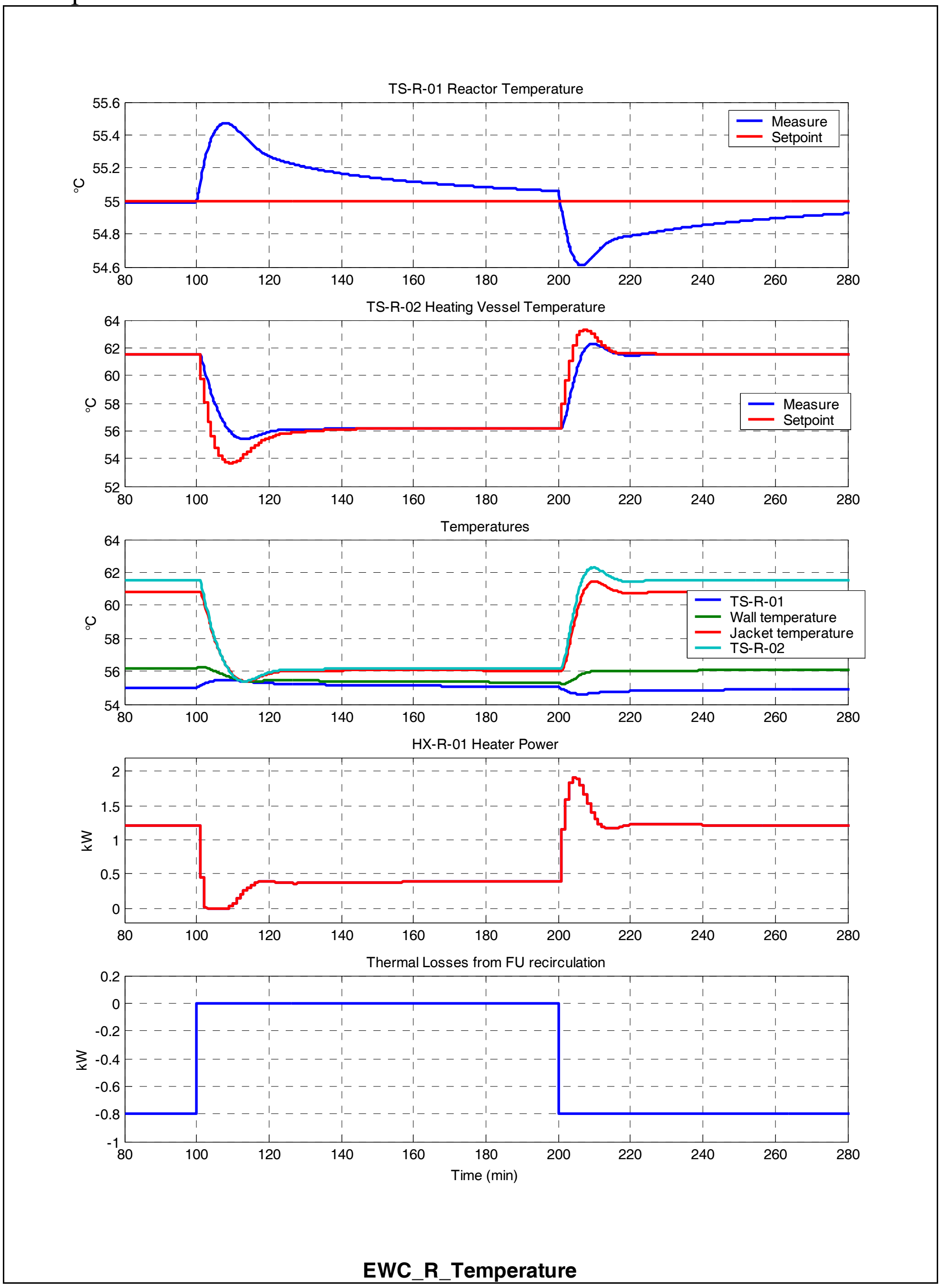


Figure 15: simulation of stop and restart of the recirculation in the filtration unit

2.3.4. Conclusion

The performed simulations show that the requirements are satisfied: the reactor temperature stays within 55±0.5°C, for the main simulated disturbances.

3. System model for bioreactor pH control

3.1. Pilot requirement

The pH must be kept between two limits:

- Too basic → methanogenesis
- Too acid → inhibition of the reaction

3.2. Process description

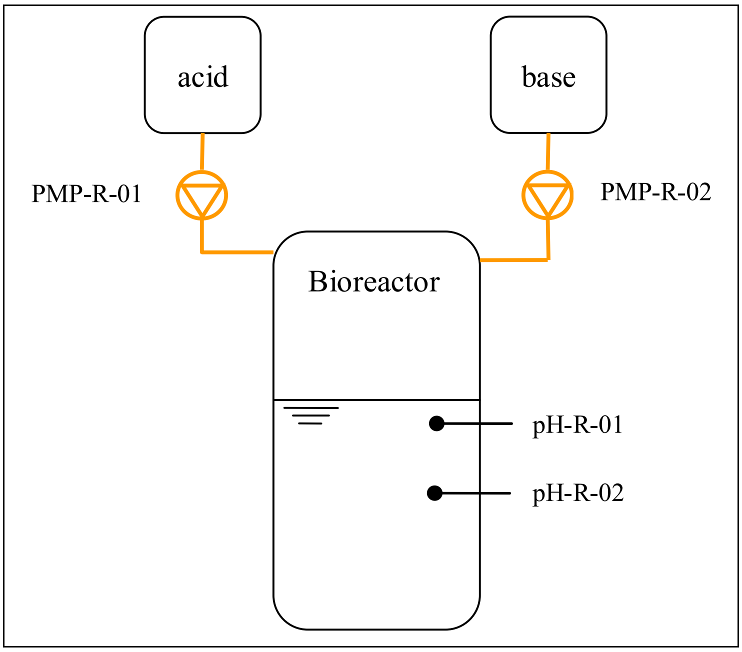


Figure 16: simplified process & instrumentation diagram for pH control

The pH is regulated by means of added strong acid (5N HCl) or strong base (5N NaOH) contained in two bottles.

3.2.1.Sensors

The pH is measured continuously by means of two probes: pH-R01 and pH-R02 (redundancy).

3.2.2.Actuators and manipulated variables

Acid or base can be added with the peristaltic pumps PMP-R-01 and PMP-R-02. Their flow rate is 1.6 ml/min.

3.2.3.Disturbances

- Influent flow rate (either acid or basic)
- The product in the reactor becomes naturally acid

3.2.4. Control

3.2.4.1. *Specification*

- Constraints:
  - 5 < pH < 7.5
  - $-\Delta < dpH/dt < \Delta$
- Set point: 5.1 < pH < 5.4 (in steady state or transient conditions)

3.2.4.2. *Control strategy*

- A split-range strategy based on a PI (Proportional Integral) regulator is implemented in the PLC.

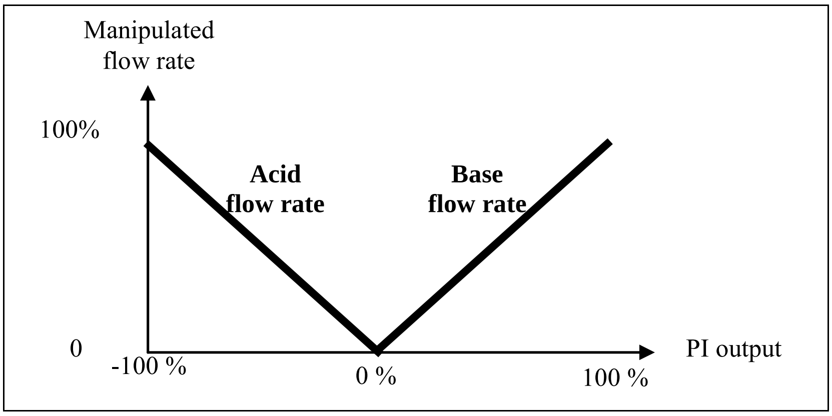


Figure 17: split-range between acid and base

- The control period is 10 min.
- An on-off control is used, by means of PWM (Pulse Width Modulators), whose maximum active times are 5 min. This prevents from continuously adding reagent. The control period is 10 min, and the active time of the PWM is limited to 5 min: so to avoid integral windup of the PI controller, the limits of the PI actions have to be ±50%.

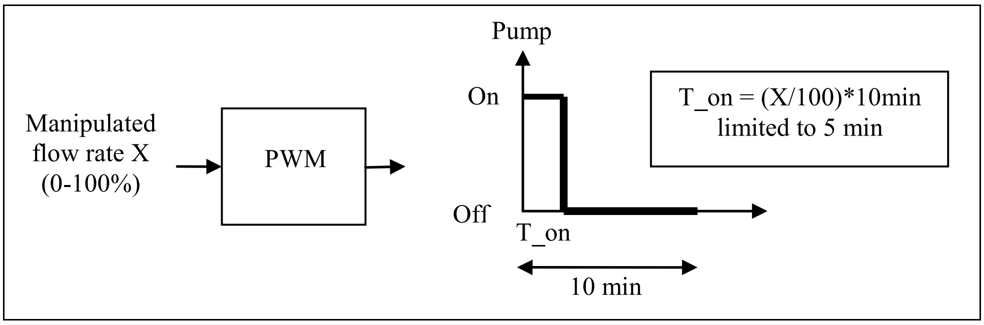


Figure 18: pH on-off control

- A dead-zone strategy is implemented. No reagent is added if the absolute value of the error between the pH and its set-point is less than the dead-zone value (typically 0.03).

3.2.4.3. *PLC code*

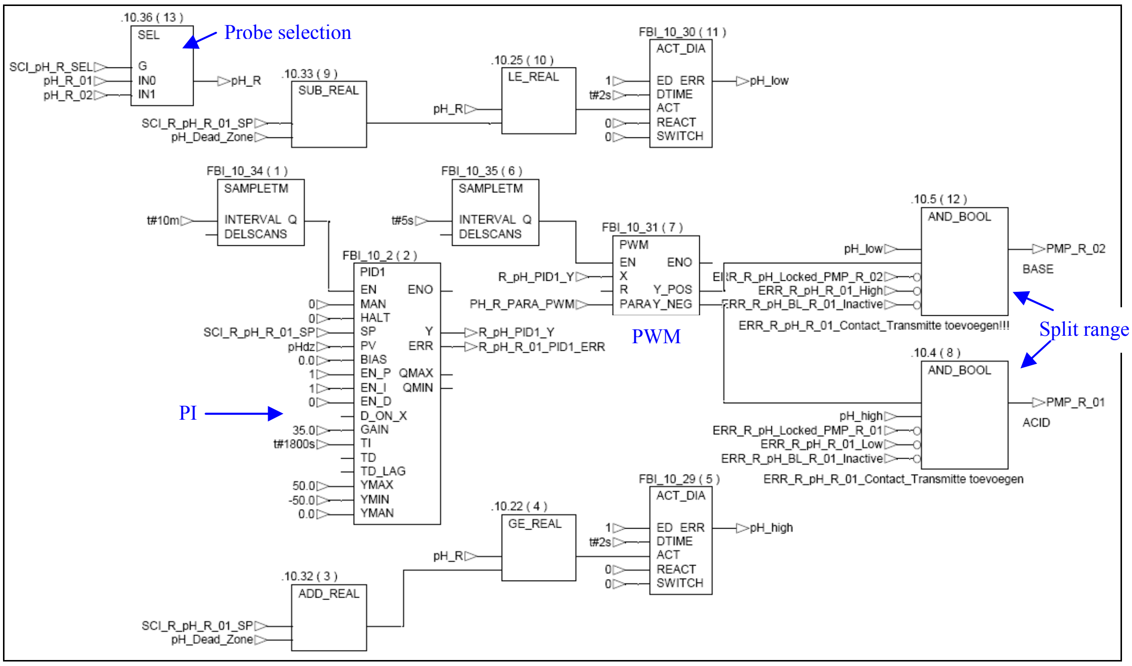


Figure 19: PLC blocks for pH control (1/2)

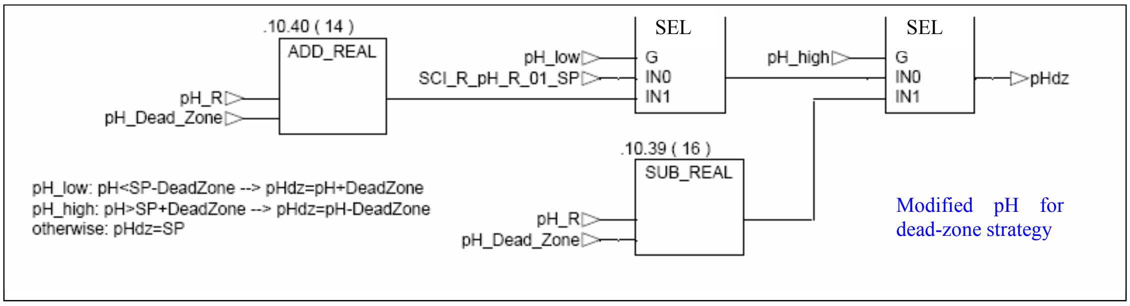


Figure 20: PLC blocks for pH control (2/2)

3.3. Model

3.3.1.Structure, equations and parameters

The pH model of the bioreactor and its environment and control is developed with Simulink.

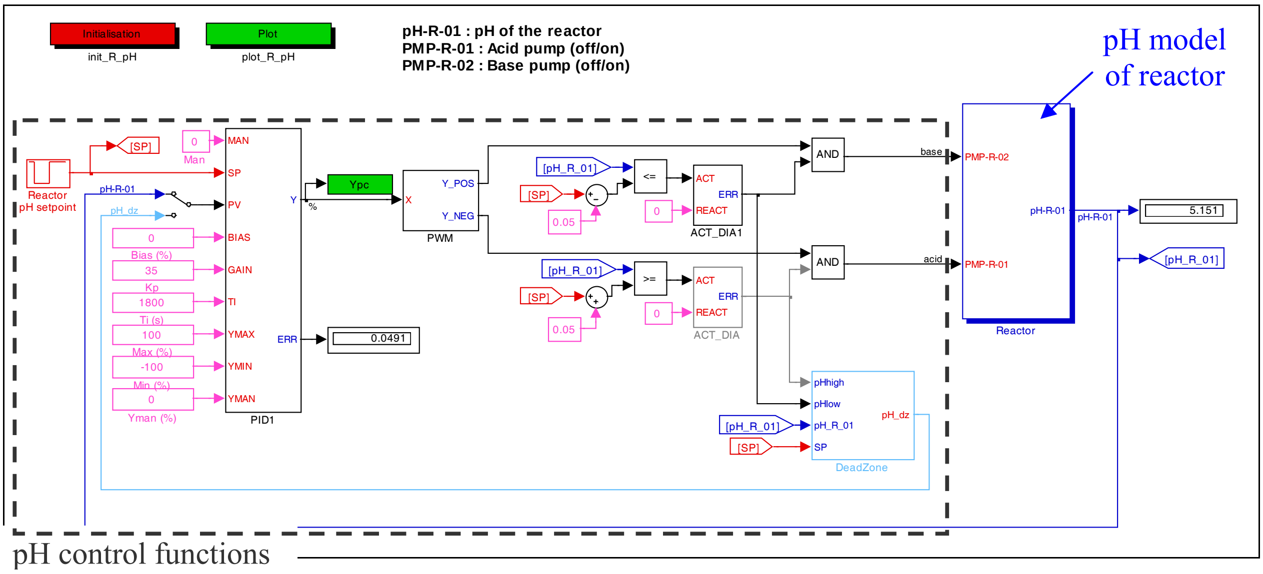


Figure 21: Simulator diagram dedicated to pH control

The simulator is made up of two parts:

- The first part replicates the control functions which are programmed in the PLC:
  - 1 PID regulator
  - 1 PWM which steers the acid pump or the base pump
  - miscellaneous blocks to handle dead-zone
- The second part models the evolution of the reactor pH with added base, acid or incoming influent product:
  - The concentration c(t) of [H^+] ions in reactor is expressed from an elementary mass balance consideration:

$$\frac{dc(t)}{dt} = \frac{1}{V} \cdot \left[q_A(t).c_A + q_B(t).c_B + q_{in}(t).c_{in} - q_{out}(t).c(t) \right] \text{ where:}$$

- c_A : excess hydrogen ion concentration of the acid reagent (5 mol/L)
- c_B : excess hydrogen ion concentration of the base reagent (-5 mol/L)
- q_A : flow rate of the acid reagent (L/s)
- q_B : flow rate of the base reagent (L/s)
- c_{in} : excess hydrogen ion concentration of the influent product (mol/L)
- q_{in} : flow rate of the influent product (L/s)
- q_{out} : flow rate of the filtrate product (L/s)

- V : volume of the reactor, considered constant (~ 100 L)

- A local experimental titration curve is used to convert the concentration c(t) to pH:

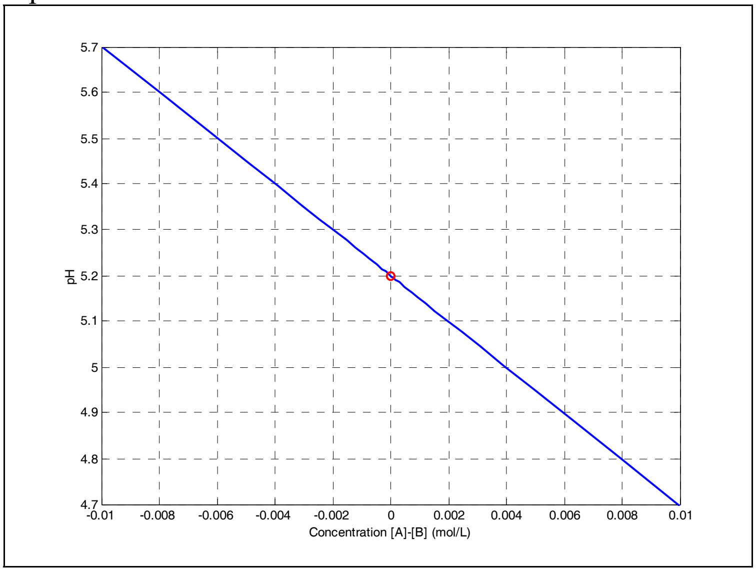
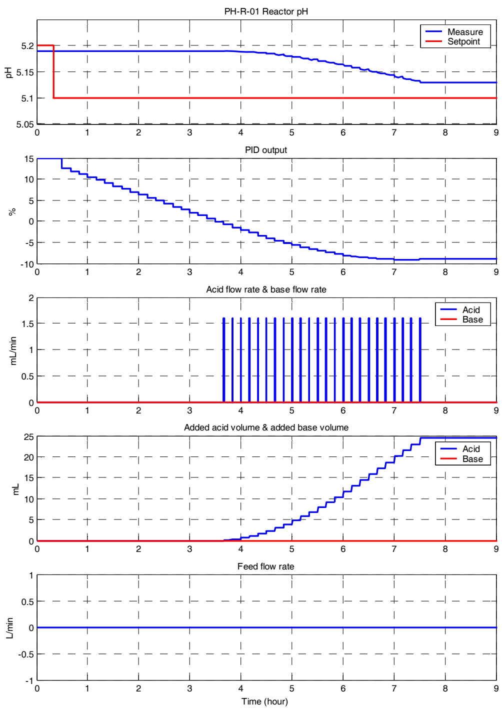


Figure 22: local experimental titration curve

The parameters are listed in appendix 8.2.

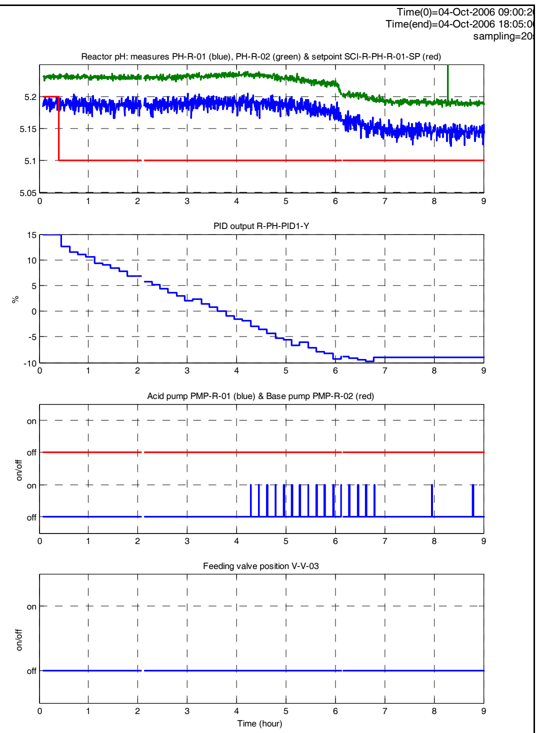
3.3.2.Validation

For a set point change of -0.1, both simulation results and process measurements give similar responses (see figures below):



EWC_R_pH

Figure 23: simulation results



EWC_R_pH: sherpa061004_3.xls

Figure 24: reactor measurements

Reactor pH responses to set point changes

3.3.3. Simulation results

Changes of set-point are simulated from an initial pH equal to 5.2. A discontinuous addition of reagent during 4 hours is required to get an incremental variation of ±0.07 for the pH (total added reagent ≈ 25 ml).

Note that every four hours, there is a disturbance due to the feeding product which is more acid in this simulation (pH=5.0).

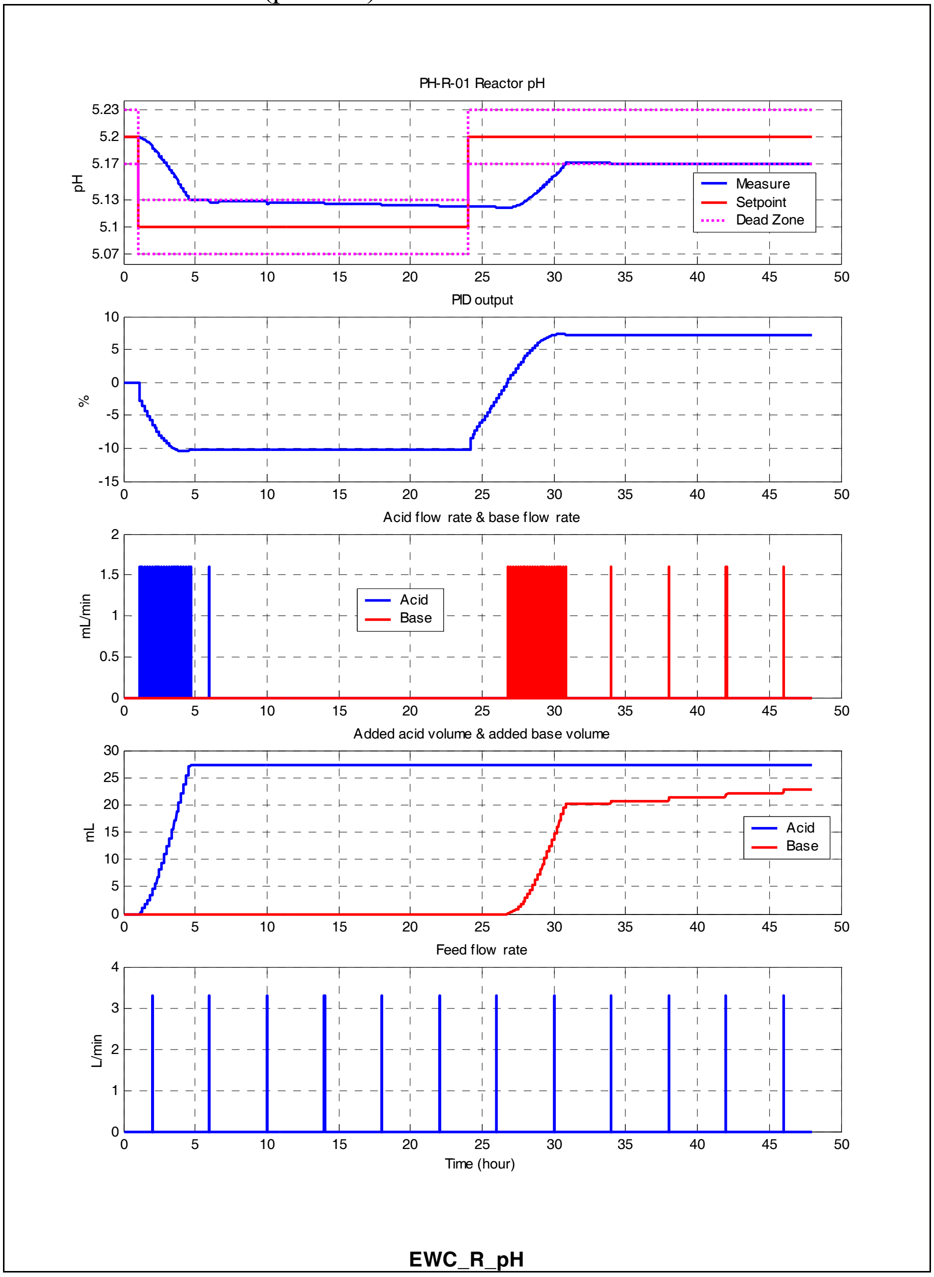


Figure 25: simulation of pH set-point changes and incoming product disturbances

3.3.4.Conclusion

The performed simulations show that the requirements are satisfied:

- the reactor pH stays close to its set-point, for the main simulated disturbance due to influent feeding;
- the rate of added reagents is small enough to have the pH move slowly to the desired value after a set-point variation or when a disturbance occurs.

4. System model for bioreactor liquid volume control

4.1. Pilot requirement

The liquid volume must be kept between certain limits for safety reason (in order not to flood the gas and gas analysis loops, and not to run the filtration loop dry). The optimal volume is near the maximum constraint (110 L).

4.2. Process description

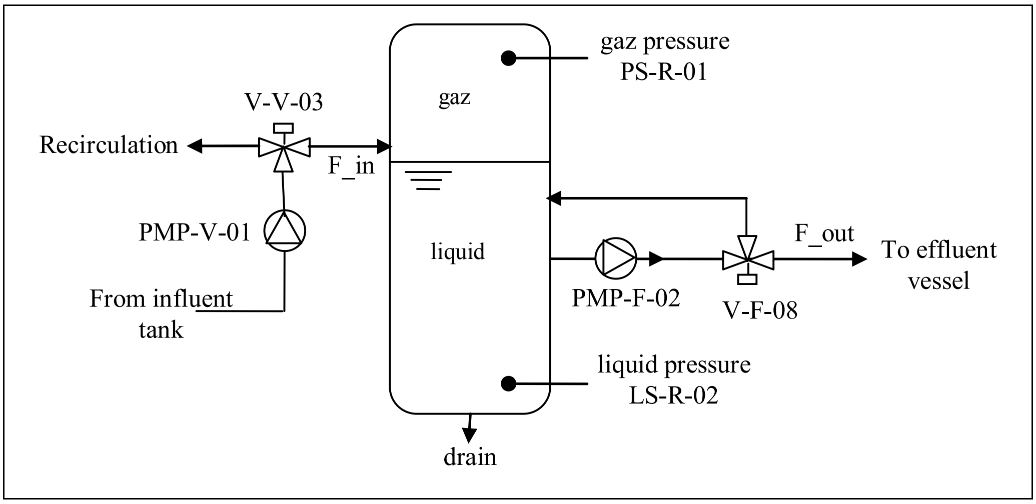


Figure 26: simplified process & instrumentation diagram for liquid volume control

The volume is regulated by feeding at regular scheduled times (every 1 hour for instance).

4.2.1.Sensors

The volume of liquid in the bioreactor (R-R-01-volume) is calculated from the pressure measurements:

- Gas pressure PS-R-01
- Liquid pressure LS-R-02

4.2.2.Actuators and manipulated variables

The volume is controlled by acting on the volumetric flow rate F_in from the influent tank to the bioreactor:

- the flow rate through pump PMP-V-01 is 3.3 L/min;
- the 3 way valve V-V-03 is switched on (i.e. flow from influent to reactor) at regular intervals of time.

4.2.3.Disturbances

The following disturbances decrease the liquid volume:

- Output flow F_out from the bioreactor to the filtration unit (continuous)
- Draining (discontinuous, happens rarely)

4.2.4. Control

4.2.4.1. *Specification*

- Nominal set point = 100 L
- Max constraint = 110 L
- Min constraint = defined by program

4.2.4.2. *Control strategy*

The volume is regulated discontinuously: at regular scheduled time (typically every 1 hour), the feeding valve V-V-03 is switched on until the calculated volume R-R-01-volume is greater than its set point SCI-V-Feed-volume-SP.

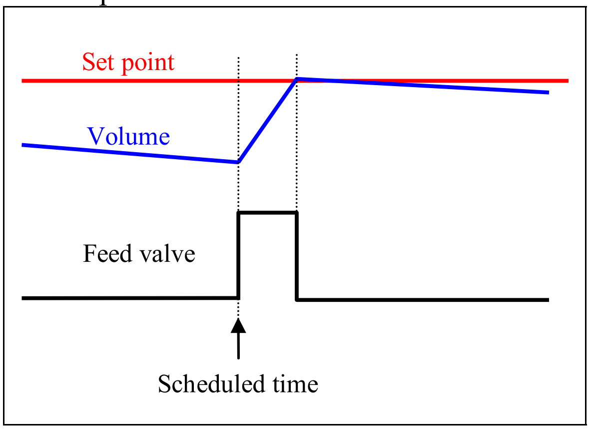


Figure 27: liquid volume control strategy

4.2.4.3. *PLC code*

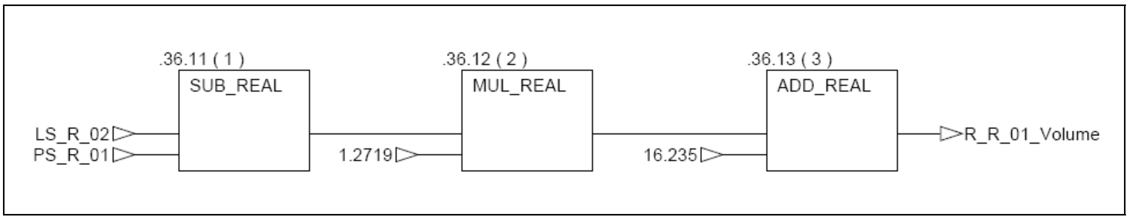


Figure 28: PLC blocks for calculation of liquid volume

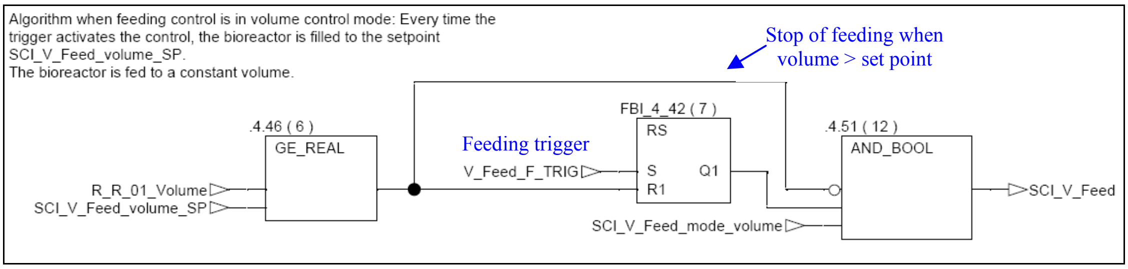


Figure 29: PLC blocks for liquid volume control (1/2)

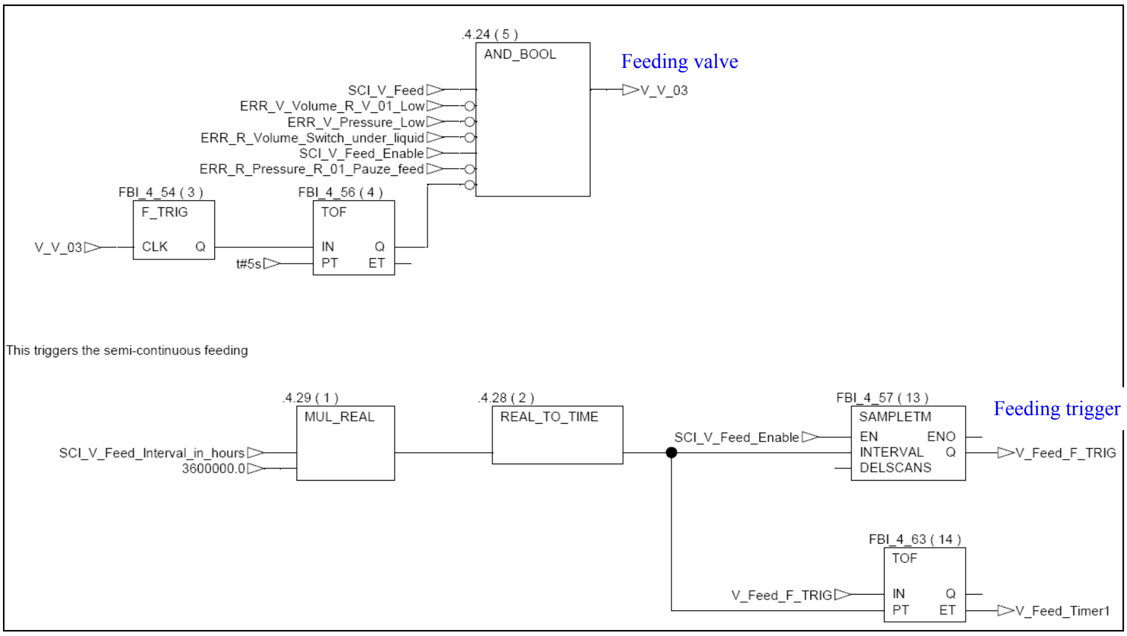


Figure 30: PLC blocks for liquid volume control (2/2)

4.3. Model

4.3.1. Structure, equations and parameters

The liquid volume model of the bioreactor and its environment and control is developed with Simulink.

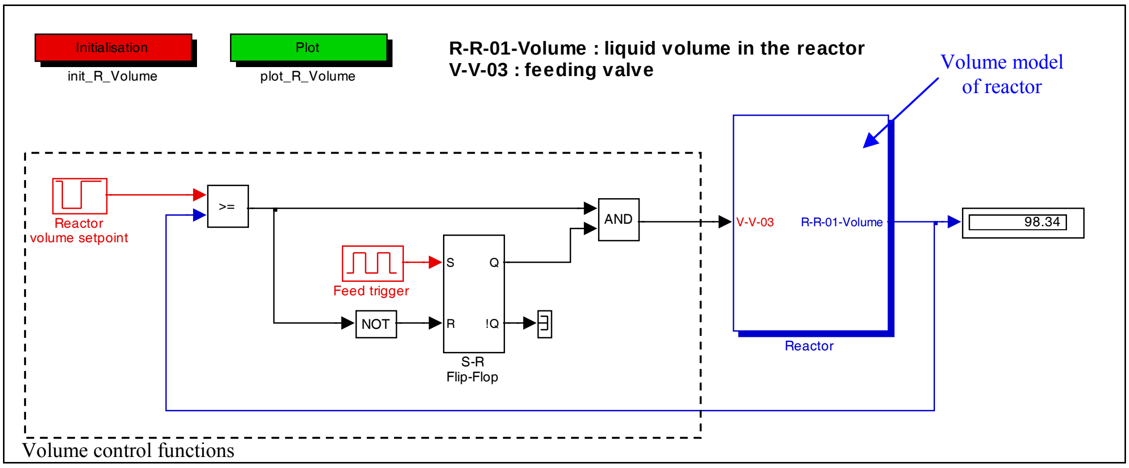


Figure 31: Simulator diagram dedicated to liquid volume control

The simulator is made up of two parts:

- The first part replicates the control functions which are programmed in the PLC:
  - feed trigger at regular intervals
  - stop of feeding when the volume measure reaches the set point

- The second part models the evolution of the liquid volume with the input flow and output flows (drain and filtrate production to the effluent vessel):

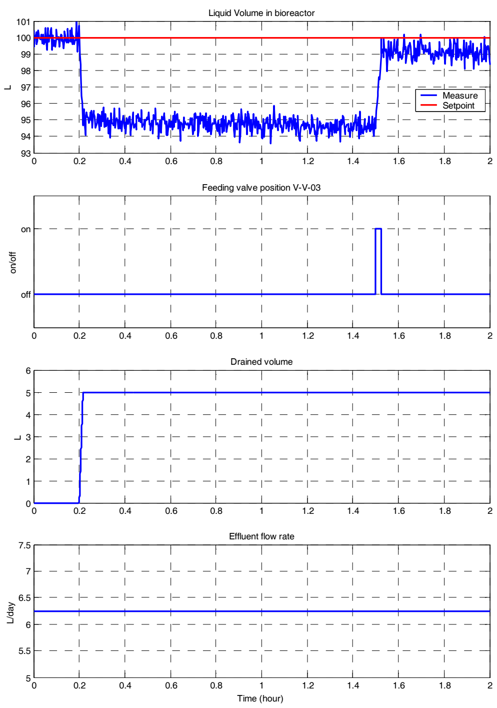
$$\frac{dV(t)}{dt} = \left[q_{in}(t) - q_{drain}(t) - q_{filtrate}(t)\right] \text{ where:}$$

  - V : liquid volume (L)
  - q_{in} : input flow when valve V-V-03 is switched on (L/s)
  - q_{drain} : drained flow (L/s)
  - $q_{filtrate}$: filtrate flow (L/s)

The parameters are listed in appendix 8.3.

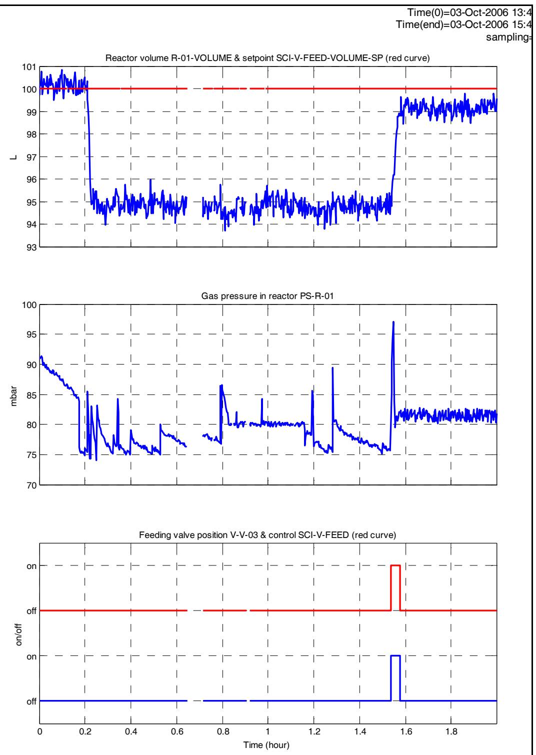
4.3.2.Validation

For a drain disturbance (~5 L), both simulation results and bioreactor measurements give similar responses (see figures below):



EWC_R_Volume

Figure 32: simulation results



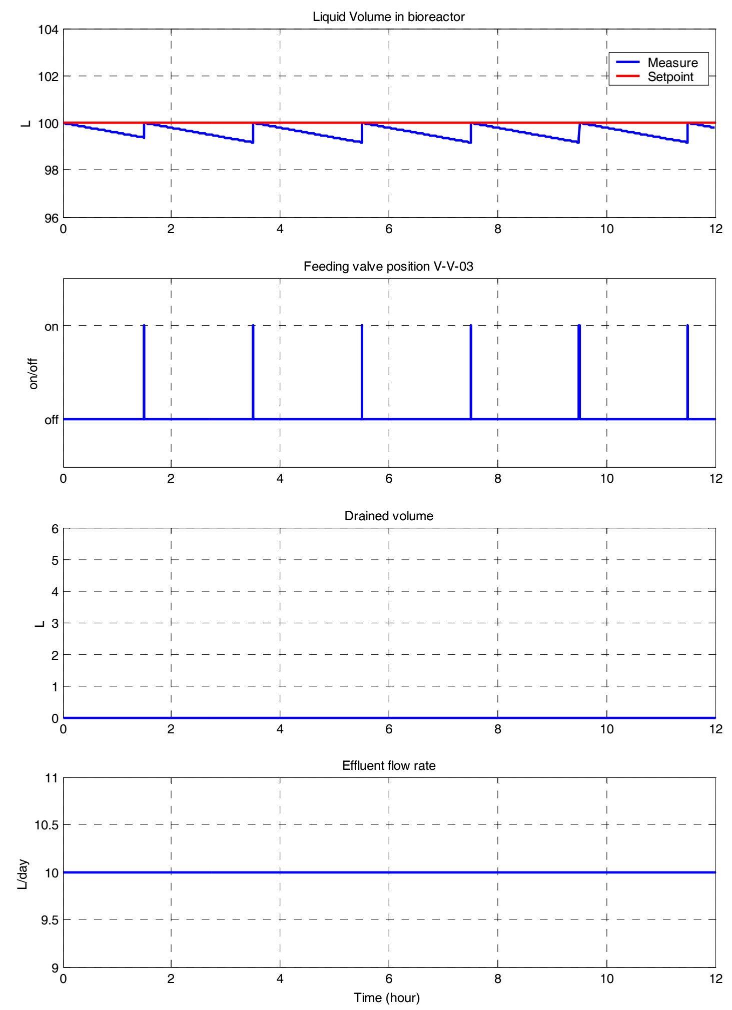
EWC_R_Volume: sherpa061003_4.xls

Figure 33: reactor measurements

Liquid volume responses to a drain disturbance

4.3.3.Simulation results

A constant output flow rate of 10 L/day is simulated. The interval of time between feeding is 2 hours. No noise is added to the measure.



EWC_R_Volume

Figure 34: simulation of liquid volume control with continuous yield

The decrease of liquid volume between two feedings is less than 1 L (which is obvious, regarding the 10 L/day yield flow rate, and the intervals of 2 hours between feedings).

4.3.4.Conclusion

The performed simulation shows that the requirements are satisfied with the volume control strategy based on feeding at regular scheduled times.

5. System model for pressure control in the gas phase of the bioreactor

5.1. Pilot requirement

A slight overpressure is required to avoid air input in the reactor.
The stability of the pressure is needed for the stability of the process.

5.2. Process description

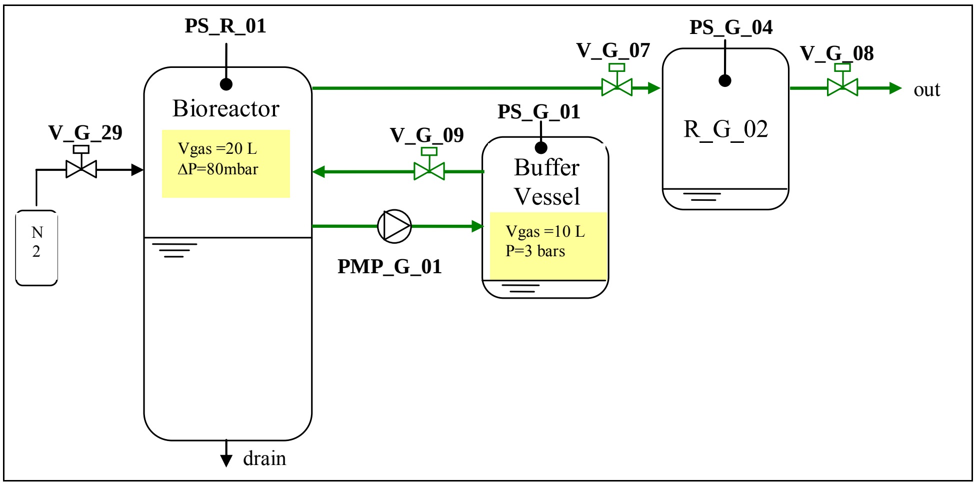


Figure 35: simplified process & instrumentation diagram for gas pressure control

The gas pressure is regulated by active and passive loops in parallel:

- Passive control:
  - flush of nitrogen N_2 into the reactor if the pressure is too low
  - release of gas outside the reactor if the pressure is too high
- Active control: an internal gas recirculation loop is used between the reactor and a pressurized gas buffer vessel

5.2.1. Sensors

The following relative gas pressures are measured:

- pressure in the gas phase of the bioreactor: PS-R-01
- pressure in the gas buffer tank: PS-G-01
- pressure in the gas outside tank: PS-G-04

5.2.2. Actuators and manipulated variables

- Flush of N2 into the reactor with valve V-G-29
- Release of gas outside the reactor with valves V-G-07 and V-G-08
- Gas flow rate:
  - from the reactor to the gas buffer vessel by mean a compressor PMP-G-01
  - or from the gas buffer vessel to the reactor via regulating valve V-G-09

5.2.3. Disturbances

- Draining which decreases the pressure
- Gas generated by the reaction
- Difference between influent and effluent flow rates (effluent is taken continuously while influent is fed at regular intervals of time)

5.2.4. Control

5.2.4.1. *Specification*

- Relative pressure set point: ~ 80 mbar
- Constraints for relative pressure: min=0, max=500 mbar

5.2.4.2. *Control strategy*

Two parallel strategies are considered:

- The passive loop is always running. The relative pressure is regulated by flushing N2 or releasing gas, when the measure reaches specified thresholds. More precisely:
  - A PID regulator is used to ensure the pressure to be higher than a set point (for instance equal to 75 mbar). When the pressure is lower than the set point, N2 is flushed into the reactor by opening V-G-29. When the pressure is higher than the set point, the valve is closed.

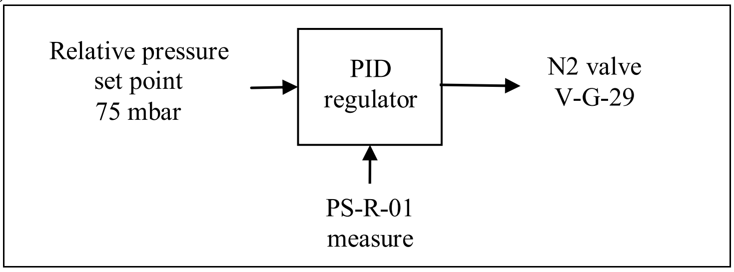


Figure 36: passive control acting on N2 flush

  - A state graph is used to ensure the pressure to be lower than a threshold (for instance equal to 90 mbar):
    - Initial state: valve V-G-08 is close; valve V-G-07 is open; pressures PS-R-01 and PS-G-04 are equal.
    - If pressure PS-G-04 exceeds threshold, V-G-07 is closed, then V-G-08 is being opened during several seconds (for releasing gas); then valve V-G-08 is closed; then valve V-G-07 is opened (to return to the initial state).

- The active loop is running when the compressor PMP-G-01 is switched on:
  - As long as the pressure PS-G-01 in the buffer vessel is lower than 3 bars, a PID regulator regulates the pressure in the reactor to a given value (for instance 80 mbar) through the valve V-G-09;
  - When the pressure in the buffer vessel exceeds 3 bars, the valve V-G-09 is manipulated (by another PID) to get the pressure in the buffer vessel back to 2.9 bars (hysteresis). In that case excessive pressure in the reactor will be reduced by releasing gas (see passive control).

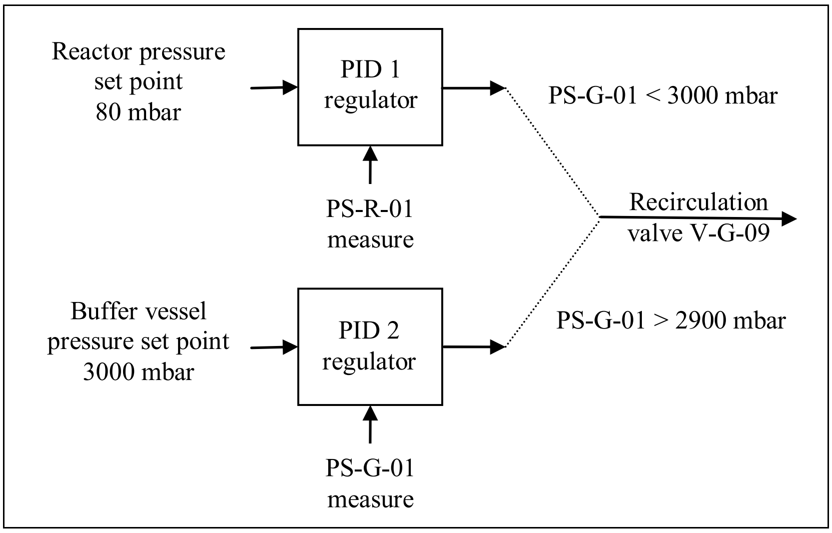


Figure 37: active loop control

- Remarks:
  - Drawback of passive control: consumption of nitrogen
  - Drawback of active control: condensation of water in the buffer and the compressor, which raises problems at start-up, noises and vibrations

5.2.4.3. *PLC code*

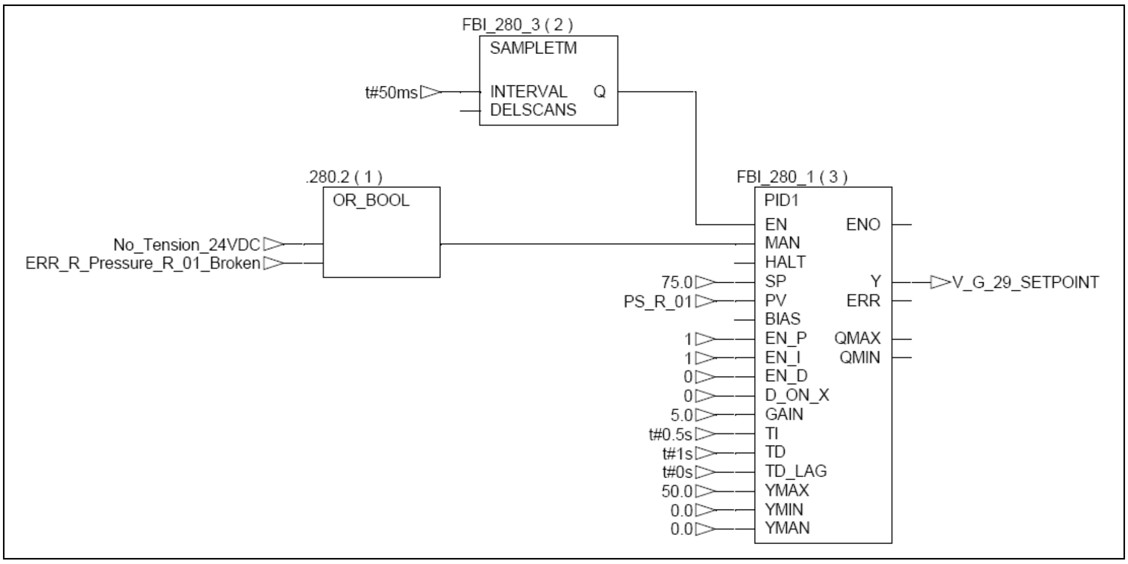


Figure 38: PLC blocks for passive gas loop: action on N2 flush valve

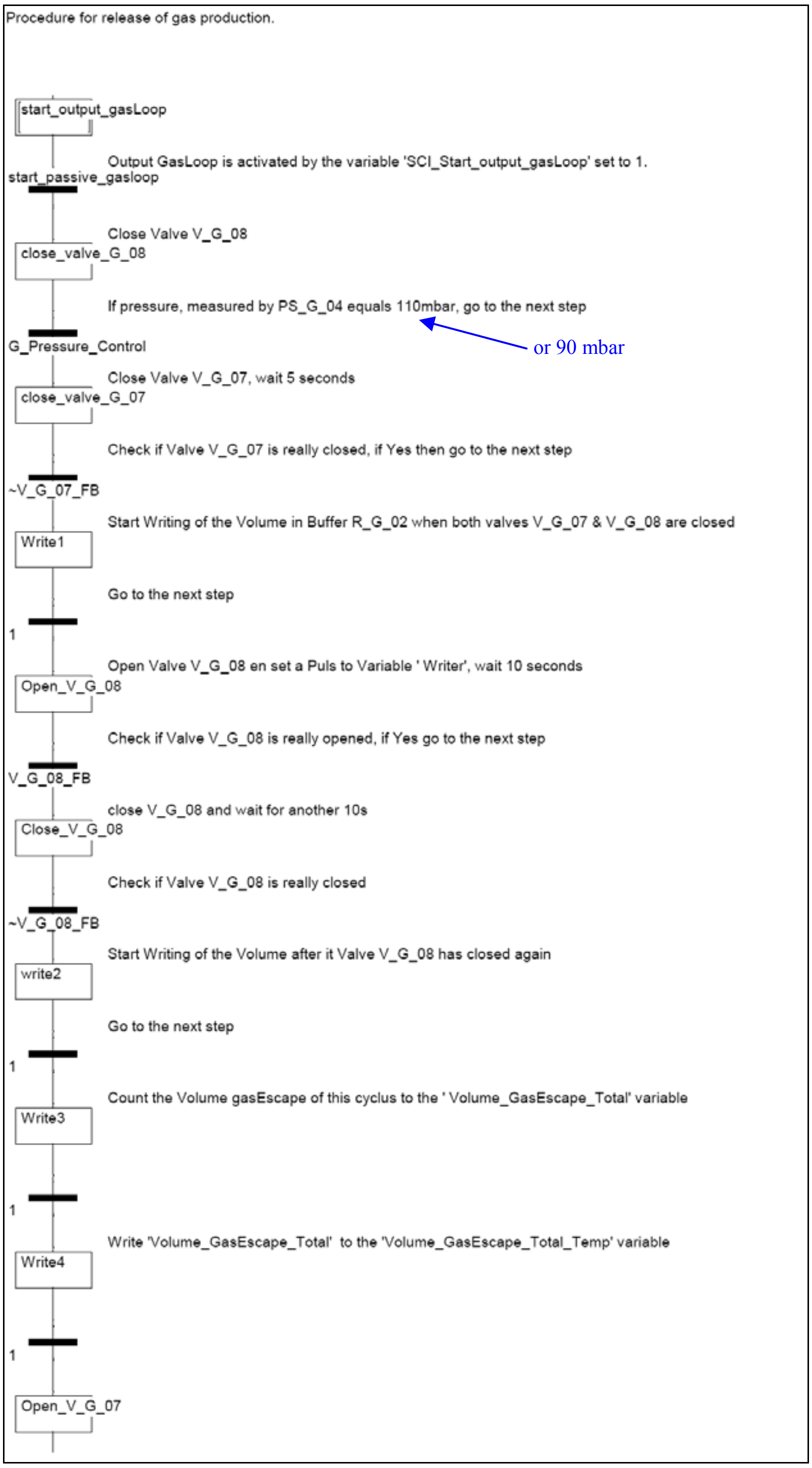


Figure 39: PLC graph for passive gas loop: action on release valves V-G-07 and V-G-08

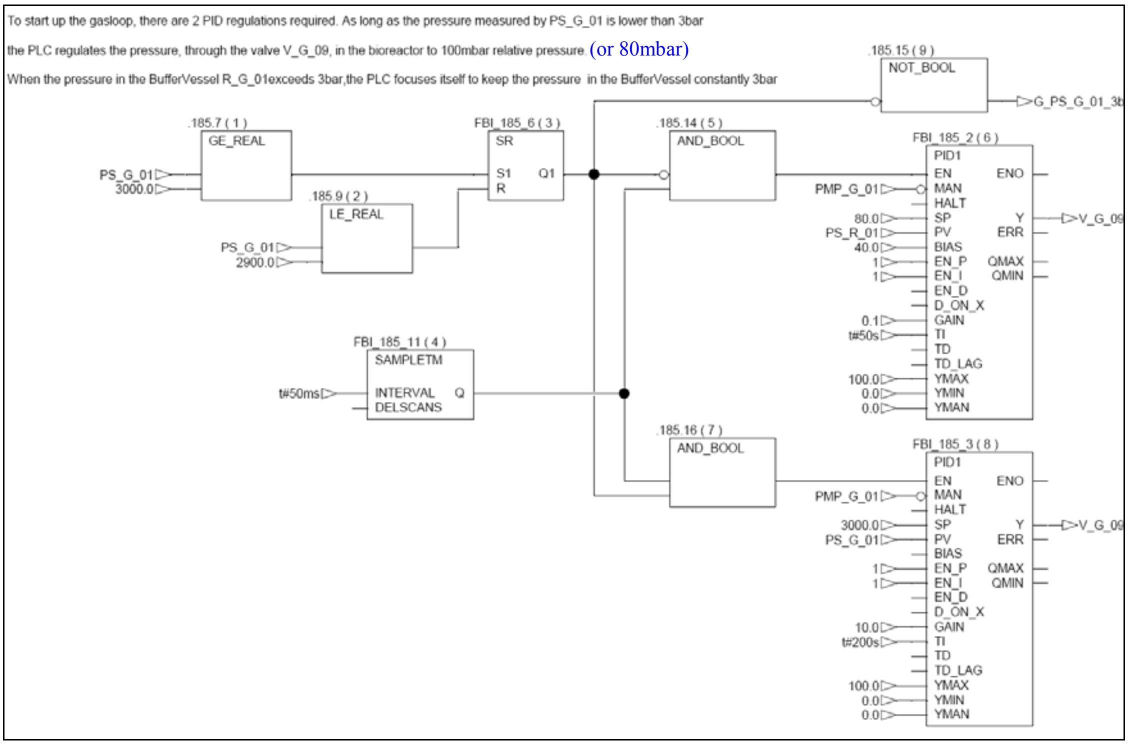


Figure 40 PLC blocks for active gas loop

5.3. Model

5.3.1.Structure, equations and parameters

The model of the gas phase in the bioreactor and its environment and control is developed with Simulink.

The simulator is made up of two parts (see Figure 41):

- The first part replicates the control functions which are programmed in the PLC:
  - 1 PID regulator and 1 graph for the passive strategy
  - 2 parallel PID regulators for the active strategy (details on Figure 42)
- The second part models the gas exchanges between the reactor, the buffer vessel, the nitrogen bottle and the exhaust compartment (see Figure 43):
  - Five gas volumes are considered (the bioreactor, the buffer vessel, the nitrogen bottle, the exhaust compartment, and a volume for the gas generated by the reaction)
  - The valves are simulated by means of pressure drops (for simplification sake, on the exhaust side, only valve V_G_08 is considered; valve V_G_07 and vessel R_G_02 are not simulated)
  - The compressor is simulated by mean of a flow source
  - The considered disturbances are:
    - Gas generated by the reaction which increases the pressure
    - Leak which decreases the pressure

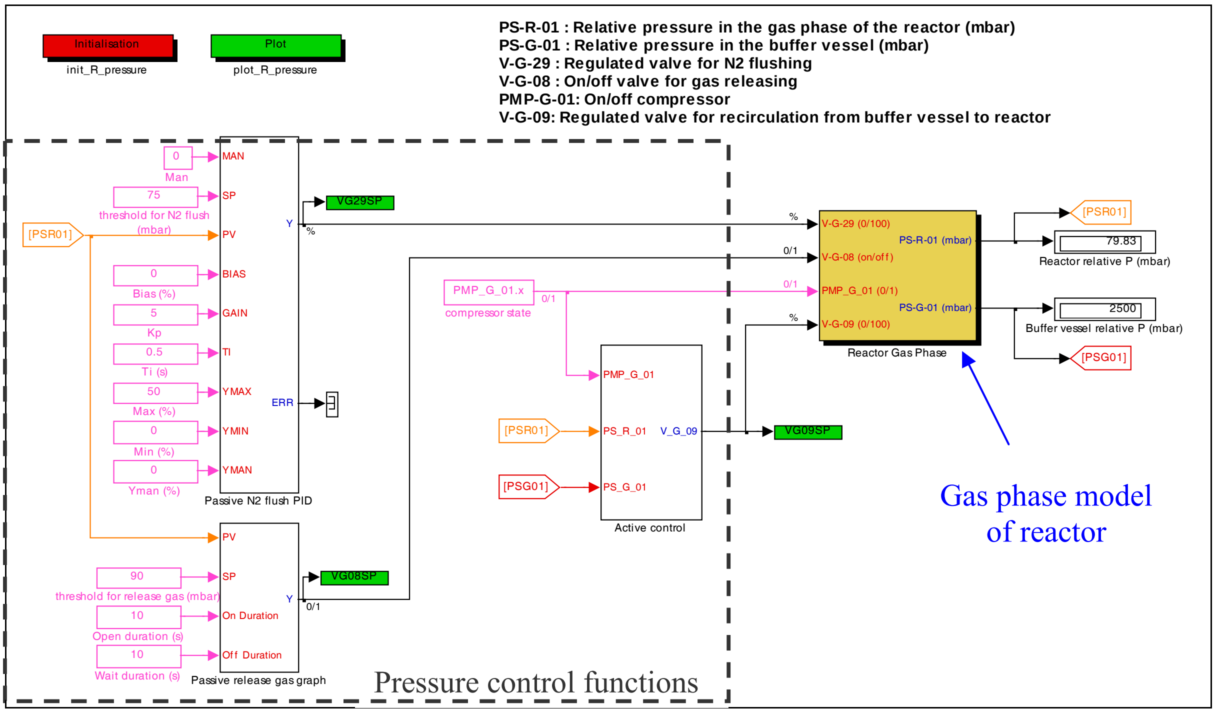


Figure 41: Simulator diagram dedicated to gas pressure control

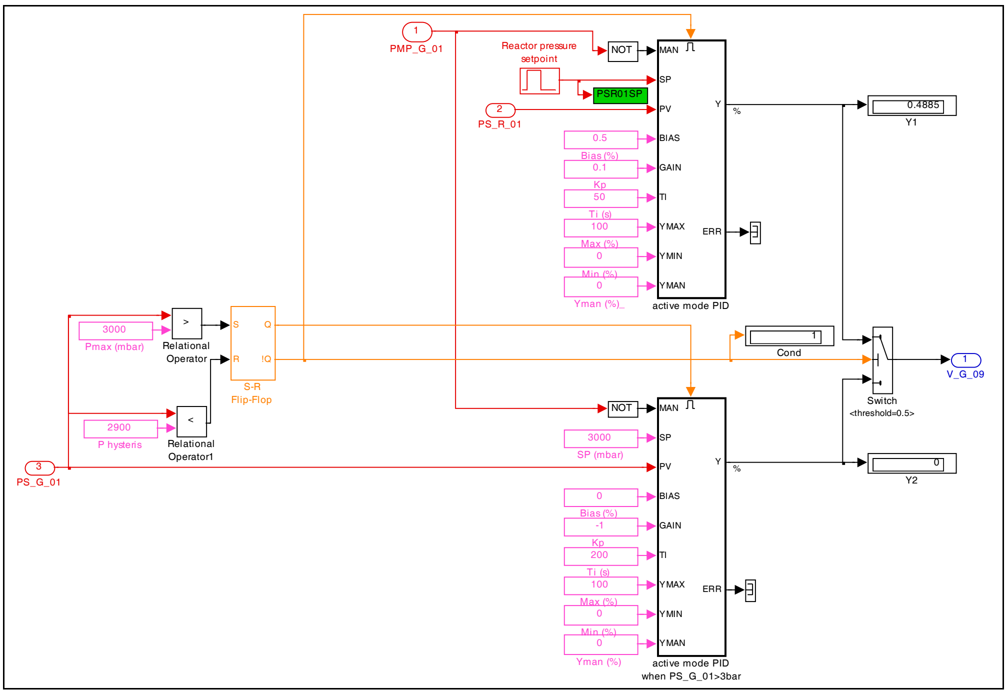


Figure 42: simulated active control

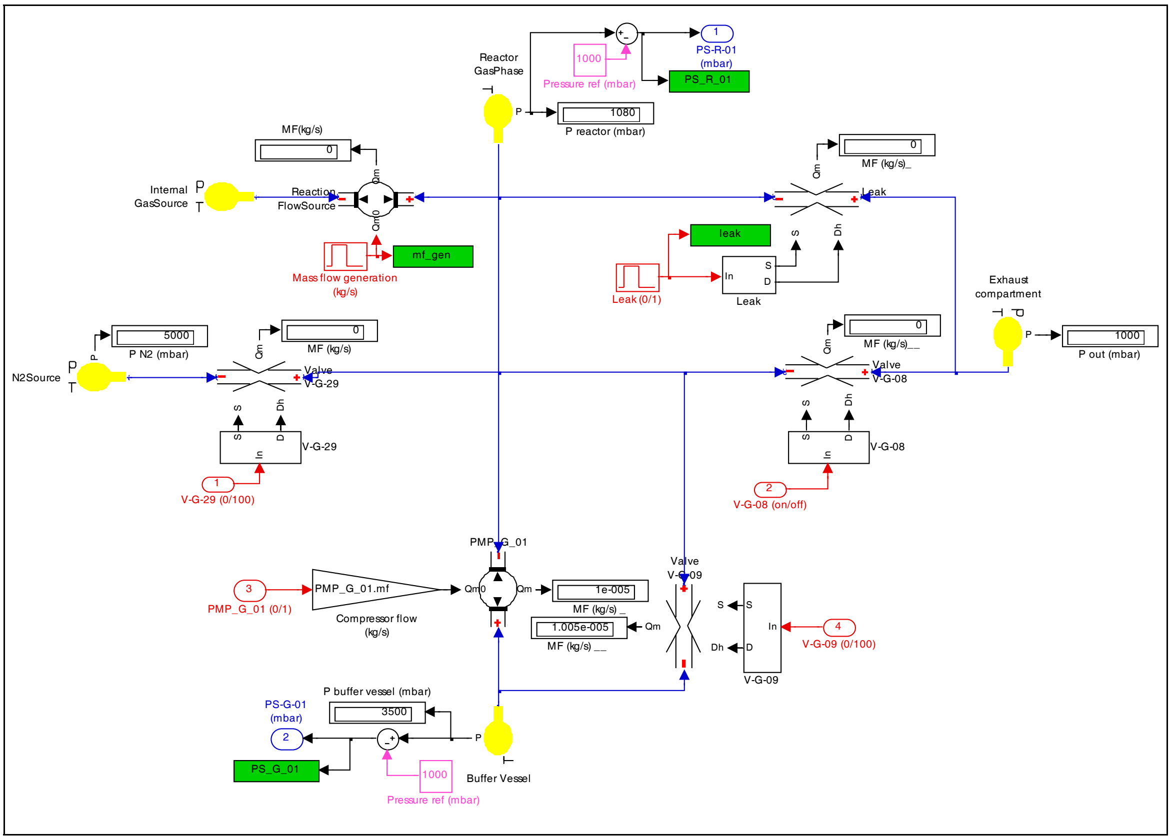


Figure 43: gas phase modelling

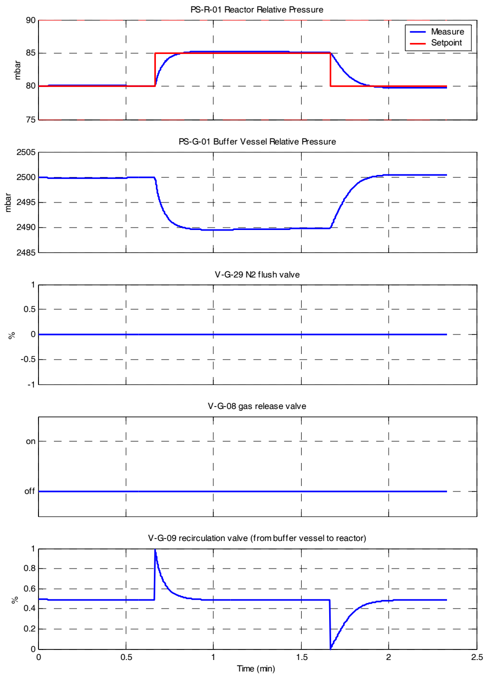
The disturbances are merely simulated by constant values, tuned to give reasonable pressure variations:

- the simulated generated gas mass flow is 10mg/s
- the leakage is simulated by an open valve with an equivalent diameter of 0.2 mm

The parameters of the simulator are listed in appendix 8.4.

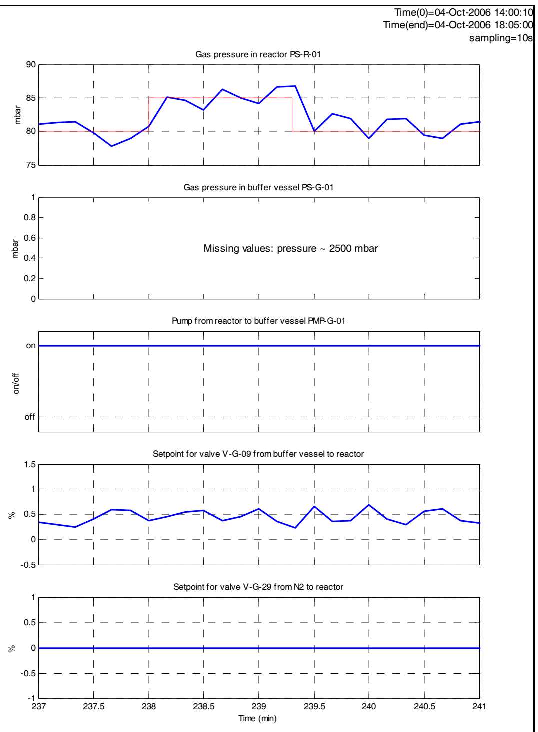
5.3.2.Validation

For a set point change of 5 mbar, both simulation results and process measurements give similar responses.



EWC_R_Pressure (active mode)

Figure 44: simulation results



EWC_R_Pressure: sherpa061004_4.xls

Figure 45: reactor measurements

Gas pressure responses to set point changes (active mode)

Remark:

- Changes of ±5 mbar is obtained within 10 seconds;
- The period of the Supervisory Data Acquisition is 10 seconds, which is too slow to get all the rapid transitions in the variables. The actual measurement period for the PLC is equal to the passive and active control period (50 ms), so the control gets the rapid transitions.

5.3.3. Simulation results

5.3.3.1. *Performances with passive strategy*

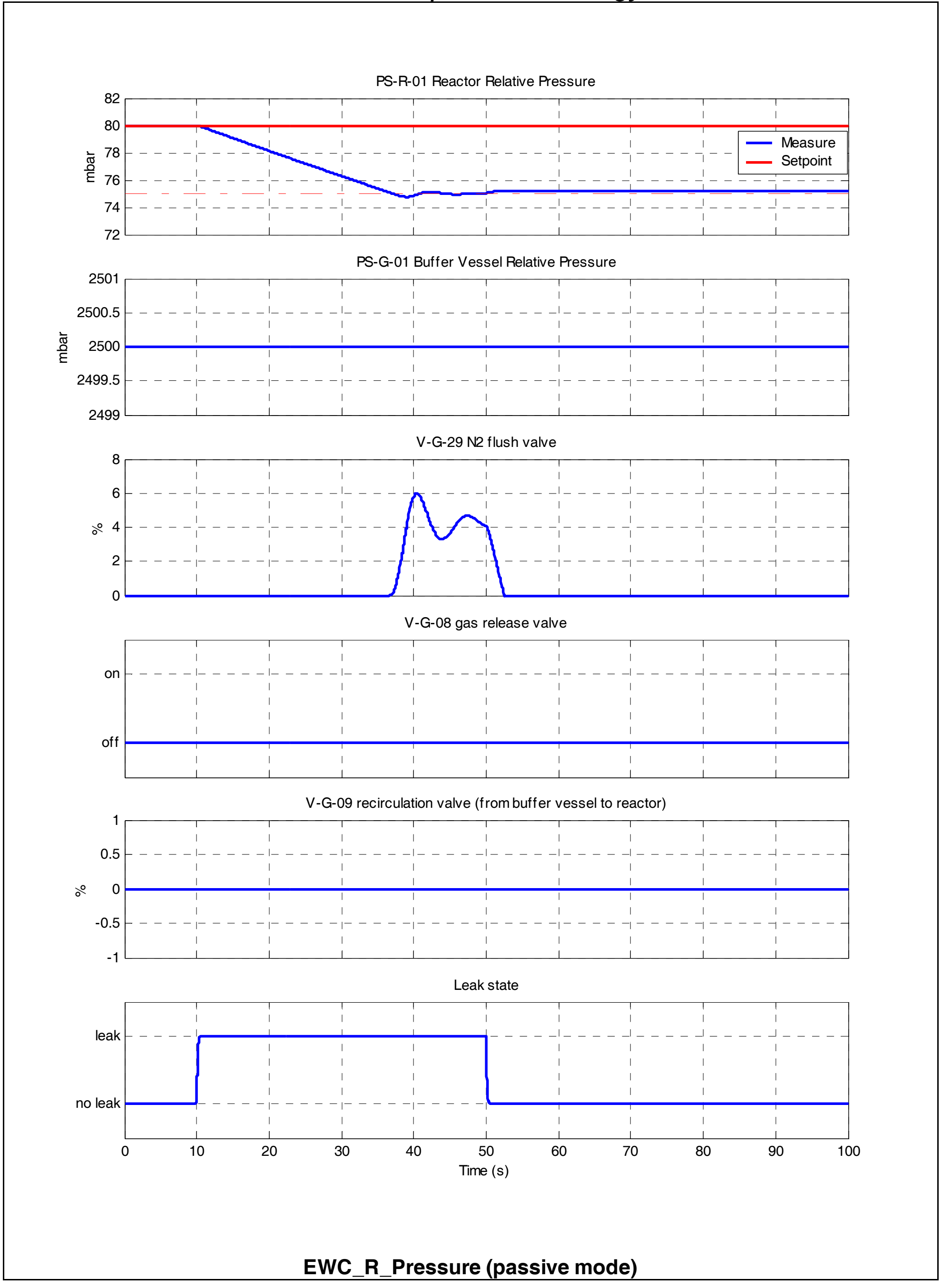


Figure 46: simulation of a leak disturbance in the context of passive strategy

Nitrogen is flushed into the reactor whenever the pressure is lower than 75 mbar.

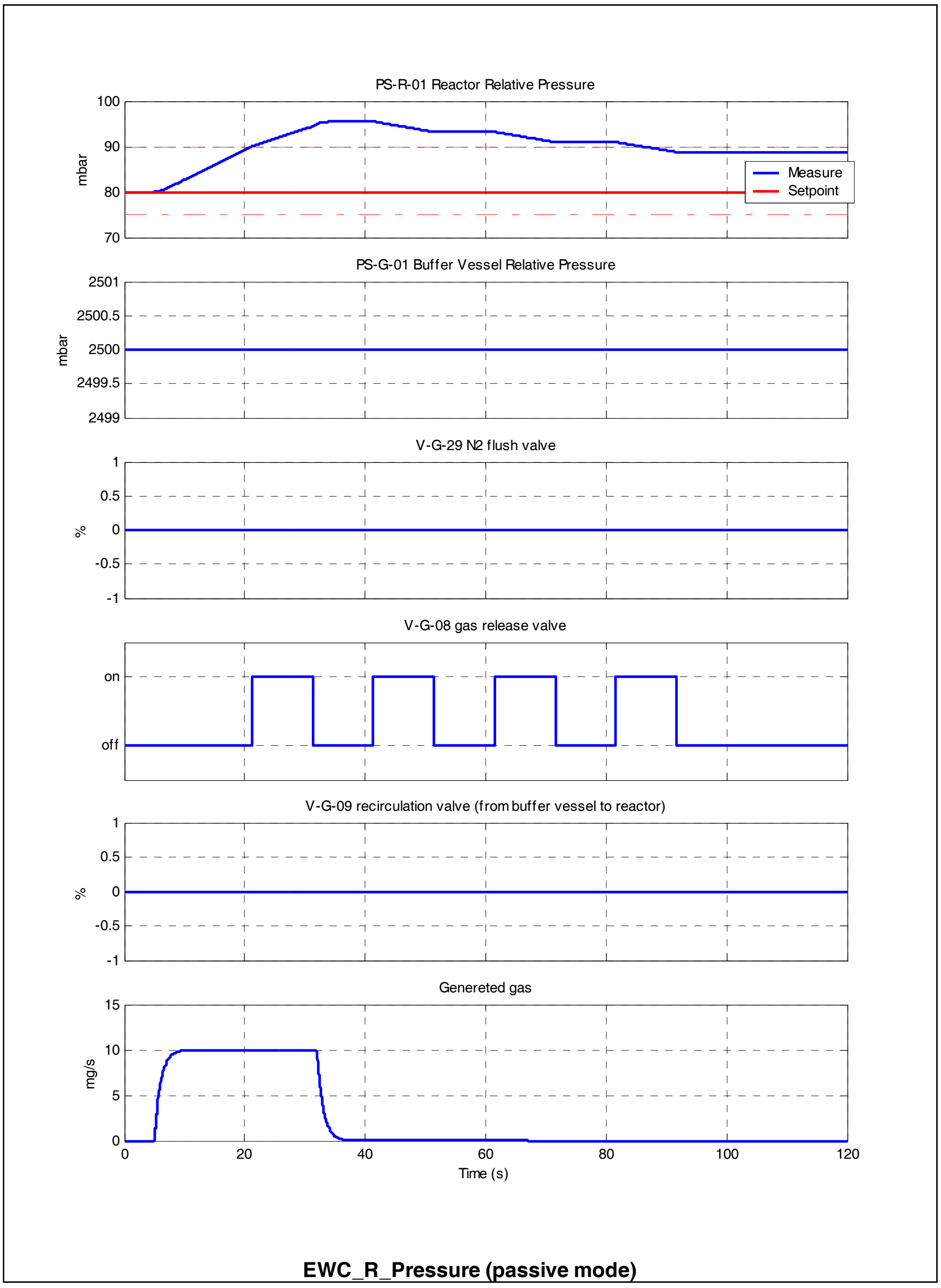


Figure 47: simulation of a gas generation disturbance in the context of passive strategy

Gas is discontinuously released outside the reactor to get the pressure lower than 90 mbar.

5.3.3.2. *Performances with active strategy*

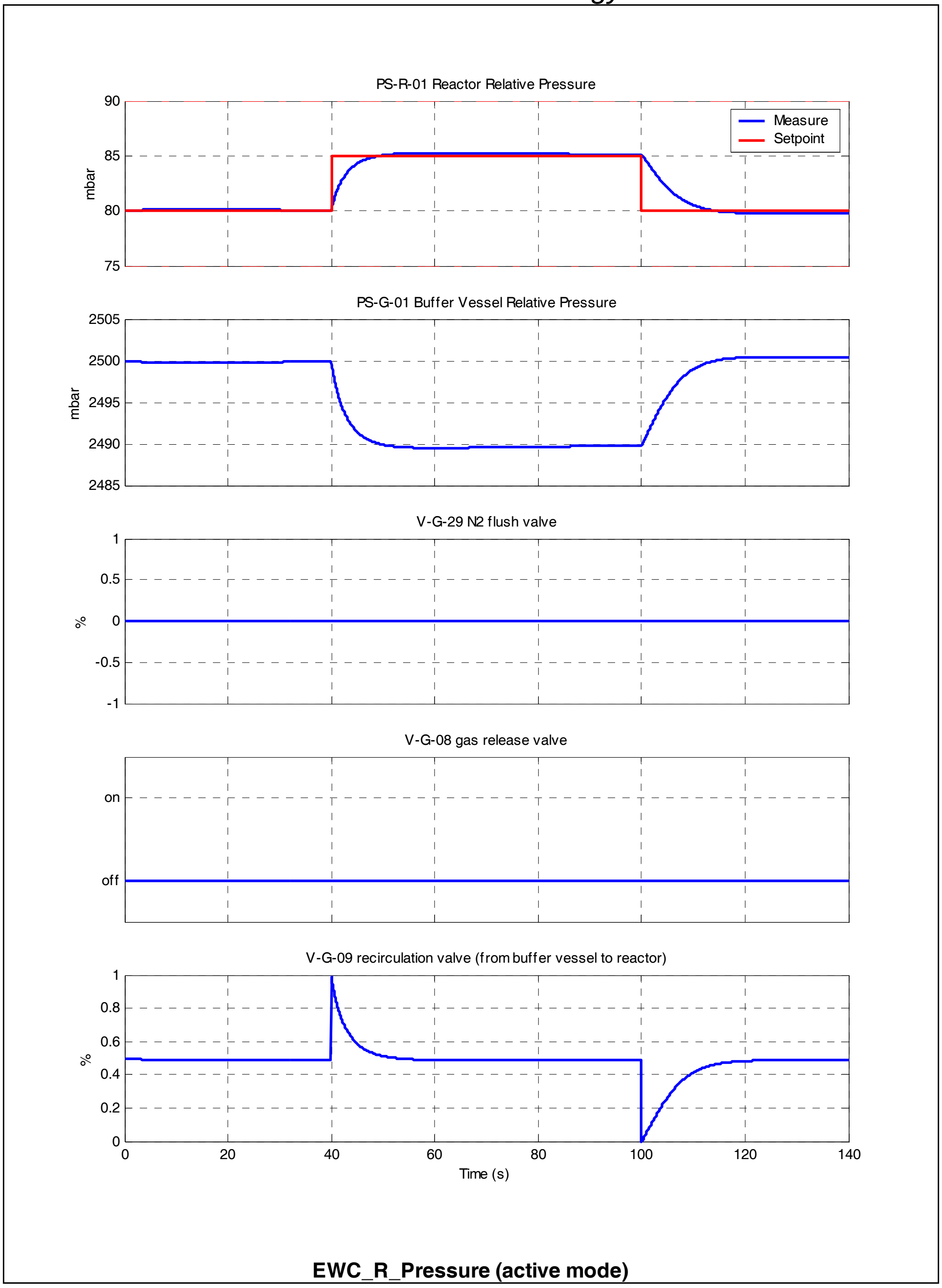


Figure 48: simulation of set point changes

The V-G-09 valve is manipulated to set the pressure to its set point. The settling time is around 10 seconds.

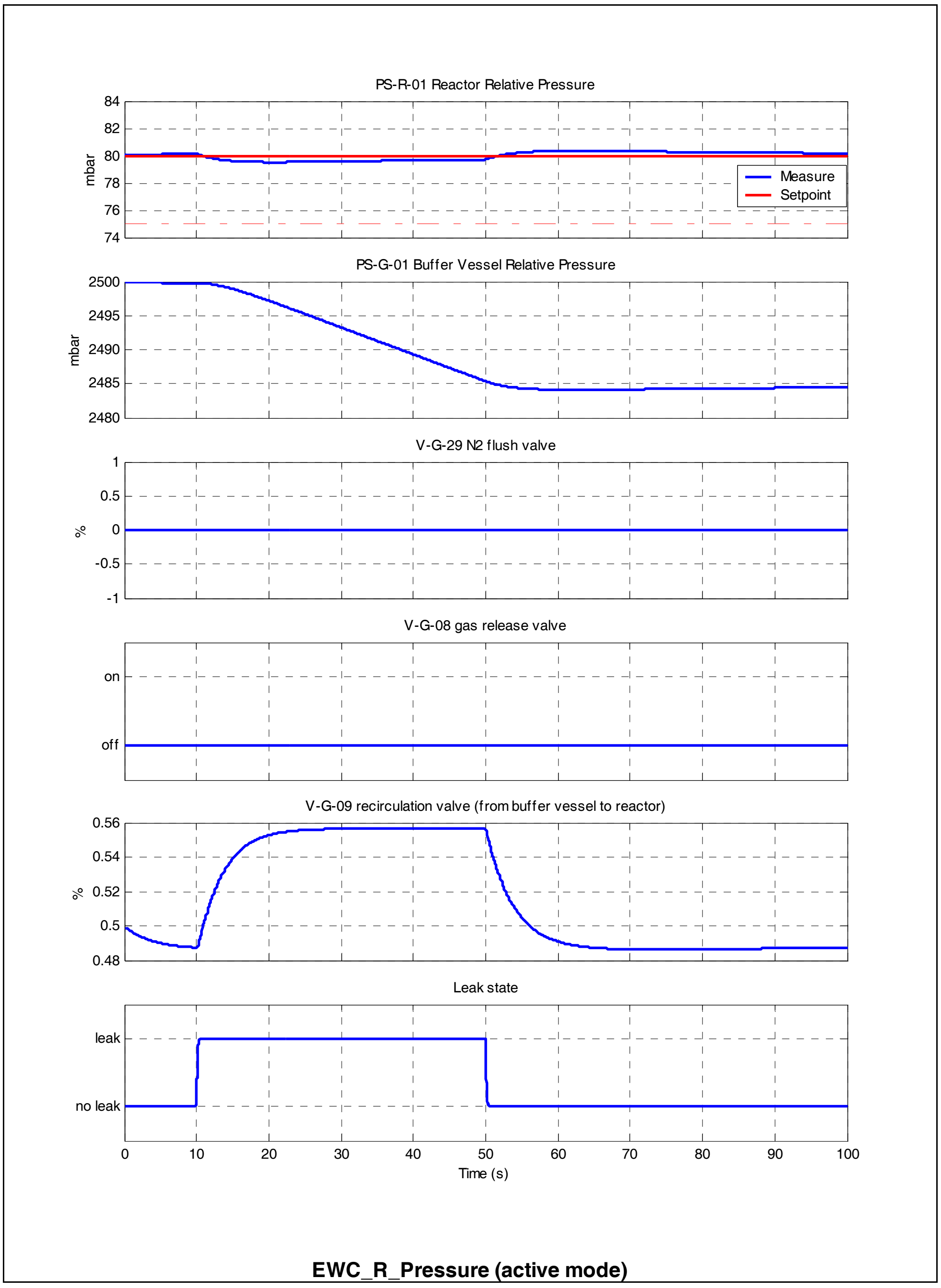


Figure 49: simulation of a leak disturbance in the context of active strategy

With the active strategy (and a pressurized buffer vessel), no nitrogen flushing is needed (compare with Figure 46).

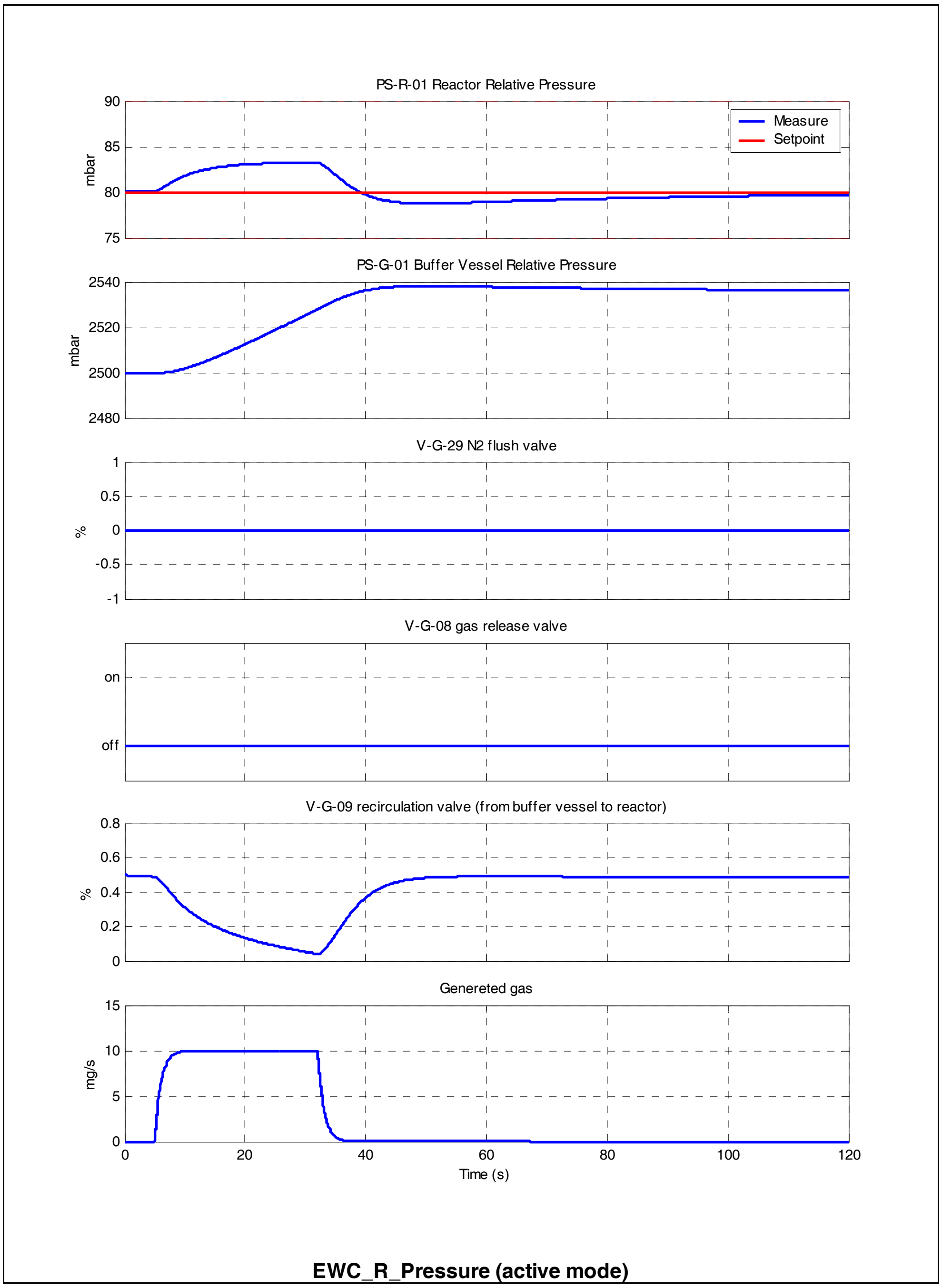


Figure 50: simulation of a gas generation disturbance in the context of active strategy

With the active strategy, no gas is released (compare with Figure 47), as long as the pressure in the buffer vessel does not exceed 3 bars.

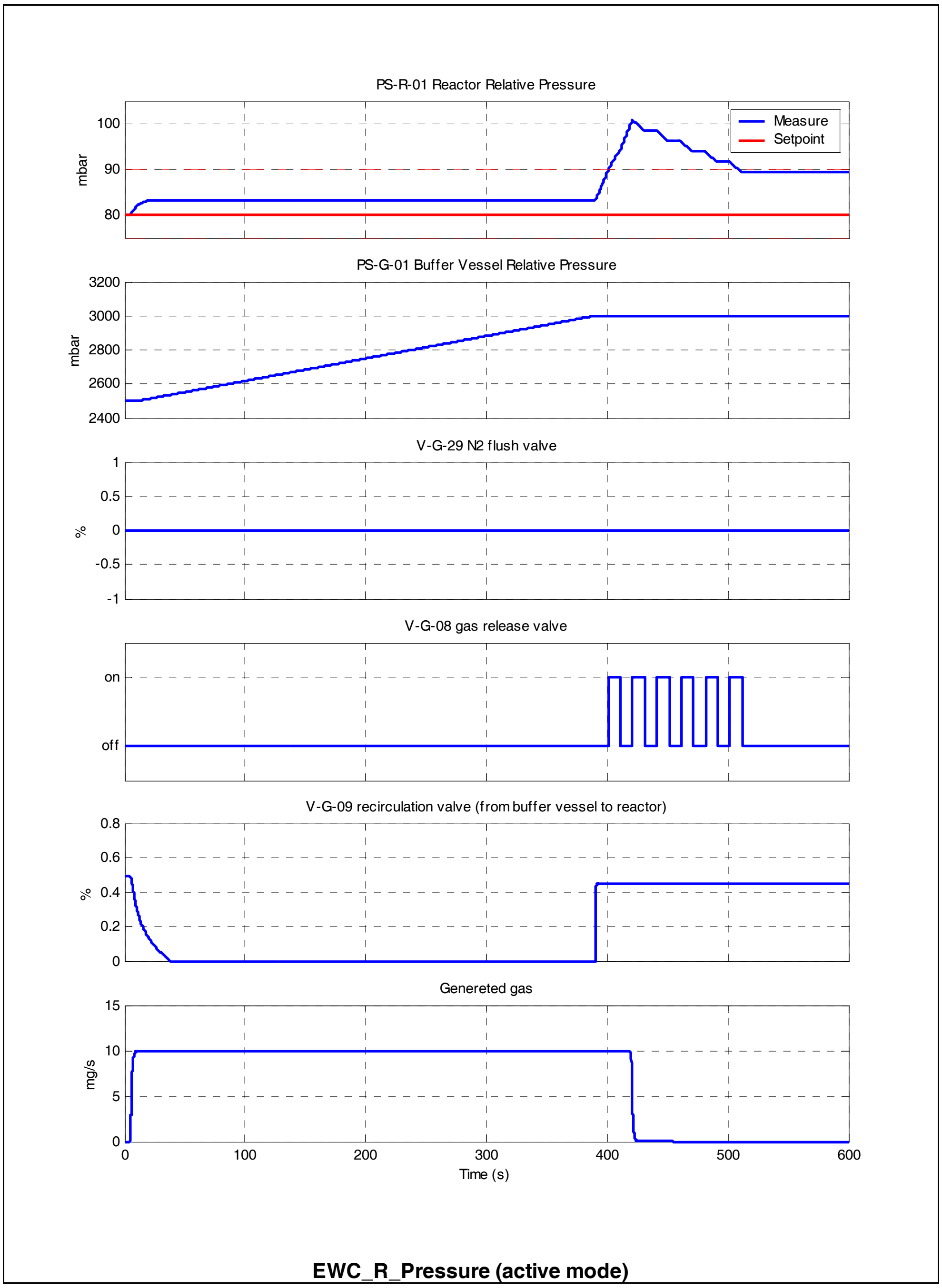


Figure 51: simulation of a gas generation disturbance with buffer vessel pressure reaching 3 bars

When the pressure in the buffer vessel exceeds 3 bars, this pressure is regulated to 3 bars, the overpressure in the reactor is then controlled by means of gas releasing.

5.3.4. Conclusion

The performed simulations show that the requirements are satisfied:

- For all the simulated disturbances, the relative pressure remains within its constraints (0-500 mbar), in both active and passive mode.
- The active mode prevents nitrogen consumption, as long as the buffer vessel is sufficiently pressurized.

Remark: The passive loop is always running; so even in active mode, N2 will be flushed into the reactor if necessary (when relative pressure lower than 75 mbar).

6. System model for temperature control in the influent tank

6.1. Pilot requirement

The temperature in the influent tank has to be controlled in order to avoid:

- chemical reaction/limit biodegradation in the tank;
- frozen products in the tank.

6.2. Process description

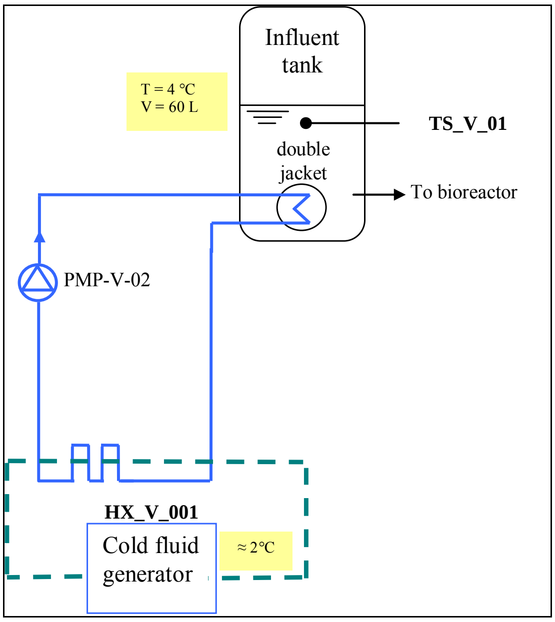


Figure 52: simplified process & instrumentation diagram for the influent tank temperature control

The temperature in the influent tank is regulated by heat transfer between the tank content and cooling fluid (glycol).

6.2.1. Sensors

Temperature in the influent tank: TS-V-01

6.2.2. Actuators and manipulated variables

The PMP-V-02 pump runs constantly (cannot be steered by the PLC). Only the cooler can be steered on/off.

6.2.3. Disturbances

The temperature of the incoming products

6.2.4. Control

6.2.4.1. *Specification*

- Set point ≈ 4°C

- Min constraint = 0.5 °C

6.2.4.2. *Control strategy*

A PID regulator is used to regulate the temperature.
The control period is 1 minute.
The output of the regulator is sent to a PWM which steers on/off the cooler.

6.2.4.3. *PLC code*

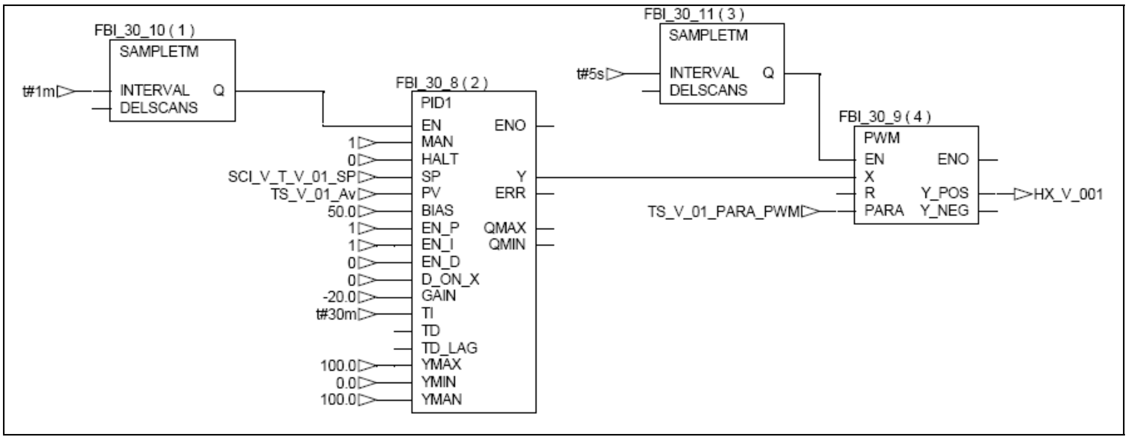


Figure 53: PLC block for influent tank temperature control

6.3. Model

No model was developed because of the non availability of data and efficient cooling fluid generator.

Nevertheless, the controller described hereinbefore (PLC code) is a standard and well known structure which will be easily tuneable with the definitive hardware.

7. Conclusion

The current study has demonstrated with the development of models that the control strategies, with their tunings, satisfied to the requirements for the process.

8. Appendix

8.1. Parameters of the bioreactor temperature control simulator

```
%ACTUATORS PARAMETERS ==================================================
% Heater HX-R-001
HX_R_001.max = 2;          % kW    % Max power

% Pump PMP-R-03
PMP_R_03.Qv = 20;          % l/mn  % Flow rate (for 1.5 m head)

%PROCESS PARAMETERS ====================================================

% Reactor -----
Reactor.Diam = 0.4;        % m     % Diameter (internal reactor diameter)
Reactor.LiquidH = 0.8;     % m     % Height of liquid
Reactor.Volume = 1000 * pi * Reactor.Diam^2/4 ...
    * Reactor.LiquidH;     % litre % Volume of liquid (~100 litres)

Reactor.Pressure0 = 1;     % bar   % Fixed pressure
Reactor.Temp0 = 55  ;      % °C    % Initial temperature

Reactor.losses = -0.15;    % kW    % Thermal losses

% Heating Vessel -----
HotVessel.Volume = 8;      % litre % Volume of liquid in hot water vessel
HotVessel.PipeDiam = 9e-3;% m      % Internal pipe diameter
                                   % (from heating vessel to reactor)

HotVessel.Pressure0 = 1;   % bar   % Fixed pressure
HotVessel.Temp0 = 61;      % °C    % Initial temperature

HotVessel.losses = -0.25; % kW     % Thermal losses

% Double Jacket -----
Jacket.Thickness = 0.01;   % m     % Thickness (of water)
Jacket.Seq = pi * ((Reactor.Diam+2*Jacket.Thickness)^2 ...
    - Reactor.Diam^2)/4;   % m2    % Equivalent section of liquid
Jacket.LiquidH = 0.5;      % m     % Height of liquid
Jacket.Volume = 1000 * Jacket.Seq ...
    * Jacket.LiquidH;      % litre % Volume of the double jacket

Jacket.Pressure0 = 1;      % bar   % Initial pressure
Jacket.Temp0 = HotVessel.Temp0;    % Initial temperature

% Forced Convection Jacket - Wall -----
FconvJW.vel = (PMP_R_03.Qv*1e-3 /60) ...
    / Jacket.Seq;          % m/s   % Fluid velocity
FconvJW.DH = Jacket.Thickness;  % m   % Hydraulic diameter
FconvJW.area = pi * Reactor.Diam * ...
    Jacket.LiquidH;        % m2    % Exchange area

% Wall (inox) -----
Wall.Thickness = 5e-3;     % m     % Thickness
Wall.Seq = pi * ((Reactor.Diam+2*Wall.Thickness)^2 ...
    - Reactor.Diam^2)/4;   % m2    % Equivalent section
Wall.Cp = 460;             % J/(kg.K)  % Heat Capacity
Wall.Density = 8400;       % kg/m3     % Volumic mass
Wall.Mass = Wall.Density * Wall.Seq ...
    * Jacket.LiquidH;      % kg    % Mass
```

```
Wall.Temp0 = Reactor.Temp0;       % Wall initial temperature

% Free Convection Wall - Reactor -----
FconvWR.DH = Reactor.Diam;% m     % Hydraulic diameter
FconvWR.area = pi * Reactor.Diam * ...
    Jacket.LiquidH;        % m2    % Exchange area

%SENSORS PARAMETERS ====================================================

%ENVIRONMENT PARAMETERS ================================================

% Influent product (semi-continously feeding) -----
Influent.Pressure0 = 1;   % bar   % Fixed pressure
Influent.Temp0 = 10;      % °C    % Fixed temperature

Influent.Qv = 3.3/60;     % l/s   % V-V-03 flow rate
                                  % (from influent tank to reactor)
Influent.Interval = 4;    % h     % Interval between 2 feedings
Influent.Amount = 6.25;   % l     % Amount by day
Influent.tp = Influent.Amount ...
    / (24/Influent.Interval) ...
    / Influent.Qv;        % s     % Feeding duration

% Recirculation from filtation -----
Filtration.losses = -0.8; % kW    % Thermal losses

%CONTROL PARAMETERS ====================================================
Reg.dt = 60;              % s     % control period
Reg.up_pos = 100;         % %     % max value for positive PWM input
Reg.tmin = 2;             % s     % minimum actuating pulse time for PWM
Reg.tmax = 60;            % s     % maximum actuating pulse time for PWM
```

8.2. Parameters of the bioreactor pH control simulator

```
%ACTUATORS PARAMETERS ==================================================
% PUMPS -----
PMP_R_01.Qv = 1.6e-3/60;  % l/s   % Flow rate of acid PMP-R-01 pump
PMP_R_02.Qv = 1.6e-3/60;  % l/s   % Flow rate of base PMP-R-02 pump

% REAGENT -----
Acid.Cu =  5;             % mol/l % excess hydrogen ion concentration
                                  % of the acid reagent
Base.Cu = -5;             % mol/l % excess hydrogen ion concentration
                                  % of the base reagent

%PROCESS PARAMETERS ====================================================
% Reactor -----
Reactor.Diam = 0.4;       % m     % Diameter (internal reactor diameter)
Reactor.LiquidH = 0.8;    % m     % Height of liquid
Reactor.Volume = 1000 * pi * Reactor.Diam^2/4 ...
    * Reactor.LiquidH;    % litre % Volume of liquid (~100 litres)
Reactor.pHinit = 5.2;             % initial pH

% Titration curve -----
delta_pH = 5.15 - 5.2;    % experimental pH variation
delta_volA = 20/1000;     % experimental added reagent (L)
delta_cA = delta_volA * Acid.Cu;
Titration.X = [-fliplr(logspace(-7,-2)) 0 logspace(-7,-2)]'; % [A]-[B] (mol/L)
Titration.pH = Reactor.pHinit + Titration.X * delta_pH / delta_cA * Reactor.Volume; % pH

Acid.eff = 1;                     % dilution effectiveness for added acid
Base.eff = 1;                     % dilution effectiveness for added base

% initial excess hydrogen ion concentration in reactor (mol/l)
Reactor.Cinit = interp1(Titration.pH,Titration.X,Reactor.pHinit);

%SENSORS PARAMETERS ====================================================
% Sensor dynamic -----
pHprobe.tau = 20;         % s     % time constant

%ENVIRONMENT PARAMETERS ================================================
% Influent product (semi-continously feeding) -----
Influent.Qv = 3.3/60;     % l/s   % V-V-03 flow rate
                                  % (from influent tank to reactor)
Influent.Interval = 4;    % h     % Interval between 2 feedings
Influent.Amount = 6.25;   % l     % Amount by day
Influent.tp = Influent.Amount ...
    / (24/Influent.Interval) ...
    / Influent.Qv;        % s     % Feeding duration

Influent.pH = 5;                  % pH of influent

% excess hydrogen ion concentration in feeding vessel (mol/l)
Influent.Cd = interp1(Titration.pH,Titration.X,Influent.pH);

%CONTROL PARAMETERS ====================================================
Reg.dt = 600;             % s     % control period
Reg.up_pos = 100;         % %     % max value for positive PWM input
Reg.up_neg = 100;         % %     % max value for negative PWM input
Reg.tmin = 2;             % s     % minimum actuating pulse time for PWM
Reg.tmax = 300;           % s     % maximum actuating pulse time for PWM
Reg.dtime = 2;            % s     % tolerance time for dead-zone
Reg.Dead_Zone = 0.03;     % -     % pH dead-zone
```

8.3. Parameters of the bioreactor liquid volume control simulator

```
%ACTUATORS PARAMETERS ==================================================
% PUMPS -----
PMP_V_01.Qv = 3.3/60;        % l/s   % Flow rate of influent PMP-V-01 pump

%PROCESS PARAMETERS ====================================================
% Reactor -----
Reactor.Vinit = 100;         % l     % Initial volume of liquid

%ENVIRONMENT PARAMETERS ================================================
% Effluent product -----
Effluent.Qv = 6.25/3600/24;  % l/s   % PMP-F-02 flow rate

% Drain product -----
Drain.Qv = 5/60;             % l/s   % drain flow rate
Drain.time = [12 13]*60;     % s     % time intervals for drain

% Sensor -----
Sensor.var = 0.15;           % l     % variance of noise

%CONTROL PARAMETERS ====================================================
SCI_V_Feed_volume_SP = 100;  % l     % volume set point
Reg.Interval = 2*3600;       % s     % Interval between 2 feedings
```

8.4. Parameters of the gas pressure control simulator

```
%ACTUATORS PARAMETERS ==================================================
PMP_G_01.x = 0;           % 0/1   % compressor state
PMP_G_01.mf = 10e-6;      % kg/s  % compressor mass flow

V_G_29.dh = 1.0;          % mm    % Equivalent diameter for V-G-29
V_G_08.dh = 0.2;          % mm    % Equivalent diameter for V-G-08
V_G_09.dh = 20.;          % mm    % Equivalent diameter for V-G-09

N2.P = 5000;              % mbar  % Nitrogen pressure

%PROCESS PARAMETERS ====================================================
% Reactor -----
Reactor.GVolume = 20;     % litre % Volume of gas

Reactor.Pressure0 = 1080; % mbar  % Initial pressure (absolute)
Reactor.Temperature = 55; % °C    % Fixed temperature

Reactor.gasflow = 1.e-5;  % kg/s  % Generated gas mass flow

% Buffer vessel -----
Buffer.GVolume = 10;     % litre % Volume of gas

Buffer.Pressure0 = 3500; % mbar  % Initial pressure (absolute)
Buffer.Temperature = 55; % °C    % Fixed temperature

%CONTROL PARAMETERS ====================================================
Reg.dtpas = 0.050;        % s     % passive control period
Reg.dtact = 0.050;        % s     % active control period
```

8.5. Document evolutions

8.5.1.Issue 1 / Revision 1

Page/Section	Comment	Answer
p 11, Section 2.3.2. Static validation	According to figure 8, the re-circulation is the sludge return flow from the filtration unit. Could you please confirm and adapt the doc?	Yes, the recirculation is the sludge return flow form the filtration unit. The doc is adapted.
p 13	Could you please add concluding remarks addressing the validity of the model to predict the behaviour of the hardware to set point changes or disturbances?	A conclusion is added addressing the capabilities of the model to predict the reactor behaviour.
p19, section 3.2.4.2, 3rd bullet	Could you please clarify the reason of the limitation of PI action? Is it because of the limited active time of the PWM?	Right: the control period is 10 min, and the active time of the PWM is limited to 5 min. To avoid the integral windup of the PI, the PI output has to be limited to 50%
p 24, figure 25	For the sake of clarity, could you please add the "+-0.03 dead zone" on the different graphs of the figure?	The dead zone is now plotted with the set point signal.
p 26, section 4.1	The liquid volume of the reactor must be kept with certain limits in order not to flood the gas and gas analysis loops, and not to run the filtration loop dry. Could you please precise these limits (110L to avoid flooding of gas loops - OK, but the low limit?)?	No information about the low limit value has been given to Sherpa.
p 27, section 4.2.4.1	Could you please give the value of the low volume defined by the program? Is it representative of the "real" low volume limit (intended to prevent the filtration loop from running dry)?	The low volume defined by the program has not been written down by Sherpa.

p 29, section 4.3.1	All the flow rates mentioned are not measured, especially the drain flow rate. Could you please clarify how these flow rates are used by the control system? In addition, Pressure measurements are used to determine the liquid volume. It would be good to include the hydrostatic pressure equation (Dp = rho.g.h) for this in the dV(t)/dt equation.	1) The flow rates mentioned are only simulated flows, and are not used by the volume control. 2) The calculation of the volume from the pressure measurements is not included in the simulation, because not necessary for control performance evaluations.
p35, section 5.3.1	Could you please clarify the equations used to model the disturbances (i.e. gas generation by bacteria and leakages)?	Actually those disturbances are merely simulated by constant values, tuned to give reasonable pressure variations: 1) for gas generation, the simulated generated gas mass flow is 10mg/s 2) for leakage, the loss is simulated by an open valve with an equivalent diameter of 0.2 mm
p38, section 5.3.2, remarks	The measurement frequency is apparently too low to get all the rapid transitions in the varaibles. Is this acceptable with respect to control of the pressure in the reactor? What can be done to improve this (hardware/Software/Code modification)?	The period of the Supervisory Data Acquisition is 10 seconds, which is too slow to get all the rapid transitions in the variables. Actually the measurement period for the PLC is equal to the passive and active control period (50 ms), so the control gets the rapid transitions.
p43, caption figure 50	Typo: passive strategy should be changed to active strategy.	Right: the caption should be "active strategy"
p45, section 5.3.4	What happens if there is for instance no pressure in the buffer (due to leak) and the active gas loop? Is the passive gas loop automatically switched on?	The passive loop is always running, so N2 will be flushed into the reactor if necessary (relative pressure lower than 75 mbar).
p47, section 6.6	Could you please precise here the amount of work to be performed in order to validate the temperature control in influent and effluent tanks?	The evaluated amount of work is: 2 days for tests & data acquisition + 2 days for analysis & reporting.