Supplementary Materials: Operator Training Simulator for an Industrial Bioethanol Plant

Inga Gerlach [1], Sören Tholin [2], Volker C. Hass [3] and Carl-Fredrik Mandenius [1,*]

1. Additional Graphical User Interfaces of the OTS

Figure S1 shows the fermentation and separation interfaces where separated biomass are collected in the tank T102 and recycled to the fermenter while the light liquid coming from the top of the centrifuges is collected in tank T101. From T101 the liquid is transferred to the mash column for distillation. Two heat exchangers provide required cooling of the streams of the system. A more detailed view on the yeast separation section is given by the third GUI (Figure S2). The distillery is shown in Figures S3 and S4: Incoming liquid from T101 is first heated by two heat exchangers and subsequent fed to the top of the mash column (MC) (Figure S3). Ethanol steam from the rectification column (RC) heats MC. Vapour is cooled and transferred to tank T004-2 that is connected to RC. The condensed ethanol steam is collected in tank T004-1 and recycled to the top of RC (reflux) (Figure S4). Water steam is used to heat the bottom fraction of RC. Ethanol steam is removed at the lower top of RC, cooled and transferred to three product tanks.

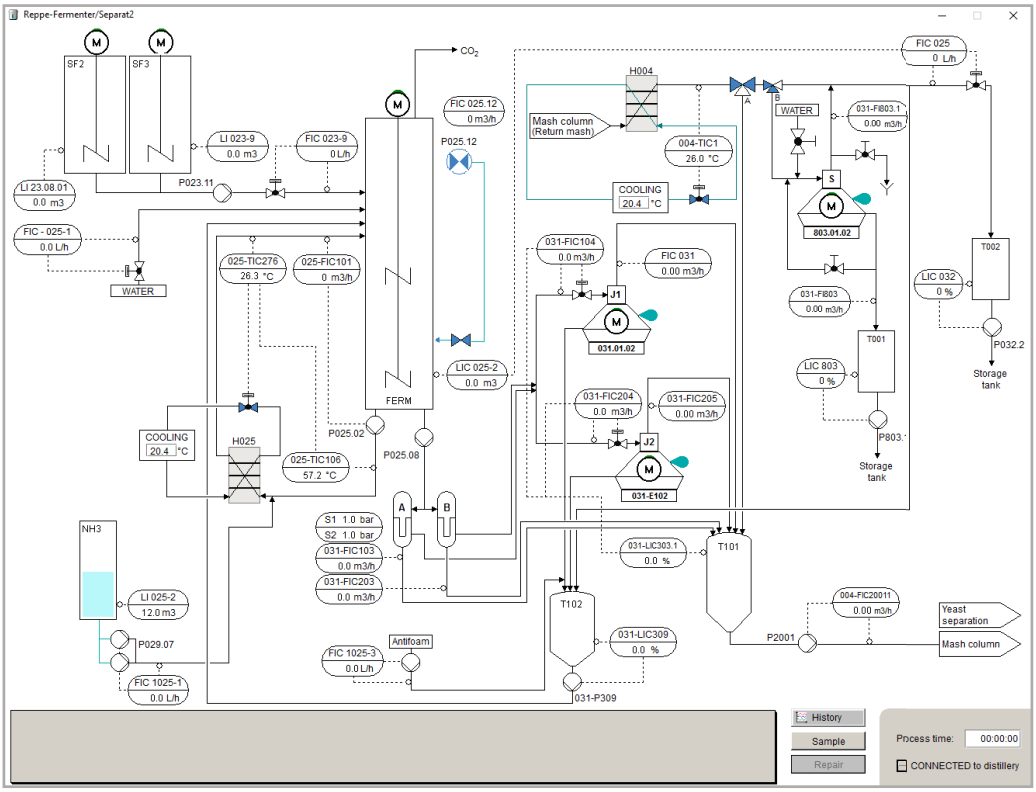

Figure S1. Graphical user interface of the fermentation and the separation process section of the OTS showing the tanks and instrumentation in an initial and inactive mode. Controllers and pumps are linked to additional sub-windows where the trainee can change controller set-points, valve configurations or start and stop a pumps and motors. GUIs of the subsequent process sections can be shown in parallel ("*Yeast separation*", "*MASH COLUMN*"). Alarm messages appear in the grey text box below.

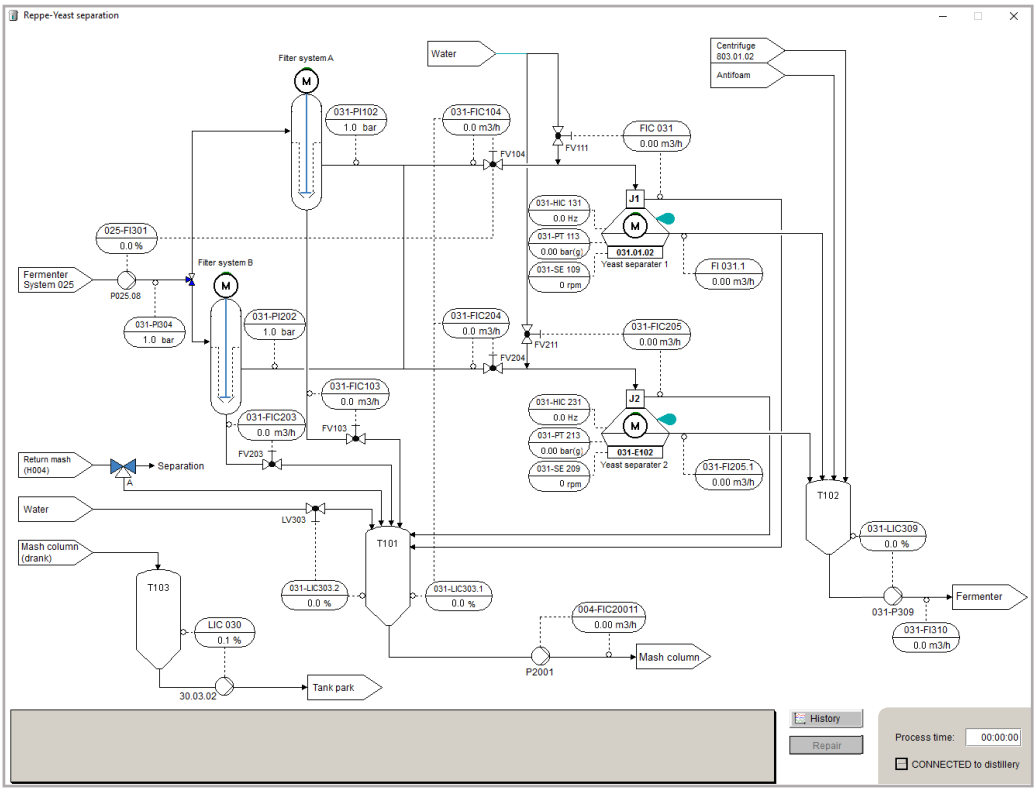

Figure S2. Graphical user interface of the separation process section of the OTS including details (cf. Figure 3) showing the tanks and instrumentation system in an initial and inactive mode. Process on-line data (e.g. pump capacities, volumes, temperatures) are shown in a separate sub-window ("History"). Alarm messages appear in the grey text box below.

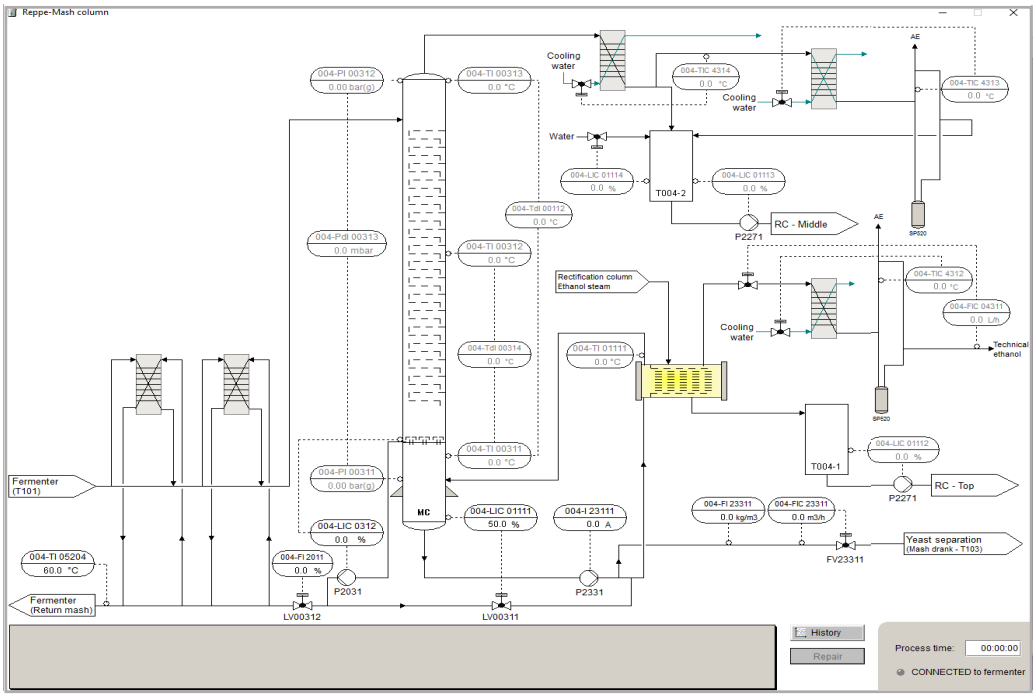

Figure S3. Graphical user interface of the distillation section in particular the mash column in the OTS showing the column, tanks and instrumentation system in an initial and inactive mode. Controllers and pumps are linked to additional sub-windows ("*History*"). GUI is linked to the GUI of the rectification column and can be opened by pushing "*RC - Middle*" or "*RC - Top*". Alarm messages appear in the grey text box below.

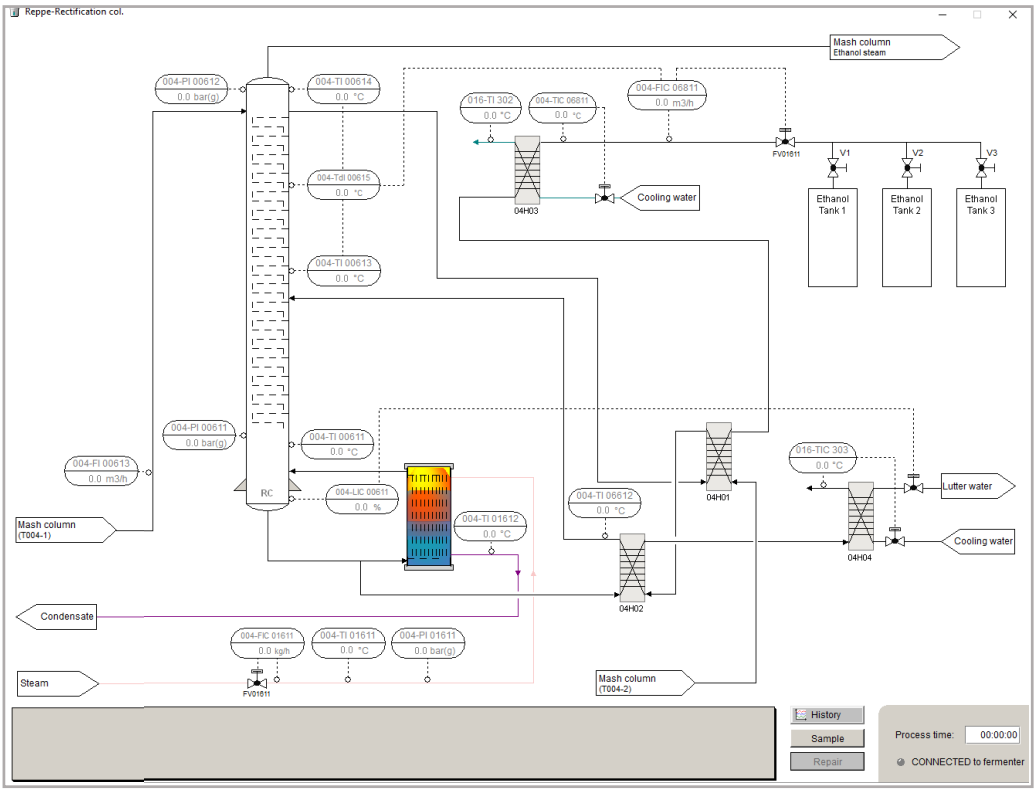

Figure S4. Graphical user interface of the distillation section in particular the rectification column in the OTS showing the column, product tanks and instrumentation system in an initial and inactive mode. Sampling is initiated in another sub-window ("Sample") where samples can be taken from the three product tanks. Process on-line data are (e.g. pump capacities, volumes, temperatures) are shown in a separate sub-windows ("History"). Alarm messages appear in the grey text box below.

2. Model State Variables for Each Sub-Model

Table S1. Overview of the state variables ($\frac{dn}{dt}$) for each sub-model.

State Variable	Pre-Treatment	Liquefaction	Saccharification	Fermentation	Filtration	Centrifugation	Distillation (MC)	Distillation (RC)	Description
c_R	●	●	●	●	●	-	-	-	Concentration of non-hydrolysable components
c_{Fi}	●	●	●	●	-	-	-	-	Concentration of fibres from flour
c_S	●	●	●	●	●	-	-	-	Concentration of starch
c_{Dex}	●	●	●	●	●	●	-	-	Concentration of dextrins
c_{Glc}	-	●	●	●	●	●	-	-	Concentration of glucose
c_{NH3}	-	-	-	●	●	●	-	-	Concentration of ammonia
c_{Pro}	-	-	●	●	●	●	-	-	Concentration of protons from acid
$c_{LF,act}$	●	●	●	●	●	●	-	-	Concentration of active LF-enzyme
$c_{LF,in}$	●	●	●	●	●	●	-	-	Concentration of inactive LF-enzyme
$c_{SF,act}$	-	-	●	●	●	●	-	-	Concentration of active SF-enzyme
$c_{SF,in}$	-	-	●	●	●	●	-	-	Concentration of inactive SF-enzyme
c_{Xact}	-	-	-	●	●	-	-	-	Concentration of active biomass
c_{XS}	-	-	-	●	●	-	-	-	Concentration of structural biomass
c_{Xi}	-	-	-	●	●	-	-	-	Concentration of inactive biomass
c_{Xd}	-	-	-	●	●	-	-	-	Concentration of dead biomass
c_{EtOH}	-	-	-	●	●	●	-	-	Concentration of ethanol
m_{H2O}	●	●	-	-	-	-	-	-	Mass of water
m_R	-	-	-	-	-	●	●	-	Mass of non-hydrolysable comp.
m_{Fi}	-	-	-	-	●	●	●	-	Mass of fibres
m_S	-	-	-	-	-	●	●	-	Mass of starch
m_{Dex}	-	-	-	-	-	-	●	-	Mass of dextrins
m_{Glc}	-	-	-	-	-	-	●	-	Mass of glucose
$m_{LF,act}$	-	-	-	-	-	-	●	-	Mass of active LF-enzyme
$m_{LF,in}$	-	-	-	-	-	-	●	-	Mass of inactive LF-enzyme
$m_{SF,act}$	-	-	-	-	-	-	●	-	Mass of active SF-enzyme
$m_{SF,in}$	-	-	-	-	-	-	●	-	Mass of inactive SF-enzyme
m_{Xact}	-	-	-	-	-	●	-	-	Mass of active biomass
m_{XS}	-	-	-	-	-	●	-	-	Mass of structural biomass
m_{Xi}	-	-	-	-	-	●	-	-	Mass of inactive biomass
m_{Xd}	-	-	-	-	-	●	●	-	Mass of dead biomass
n_{H2O}	-	-	-	-	-	-	●	●	Molar concentration of water
n_{EtOH}	-	-	-	-	-	-	●	●	Molar concentration of ethanol
DO	-	-	-	●	-	-	-	-	Dissolved oxygen
V	●	●	●	●	●	●	●	●	Volume
T	●	●	●	●	-	-	●	●	Temperature
y_{PI}	-	-	-	-	-	-	●	●	Control error over the time to simulate vapour rates

3. Standard Operation Procedure for starting the hydrolysis section of the OTS

Table S2. Standard Operation Procedure (SOP) for starting the hydrolysis section of the bio-plant.

Step	Procedural Action in the OTS	Handling the OTS ("Button"/Figure/Controller Set Point/Controller Values)
1	Start the program Reppe-OTS.	Start WinErs using the Reppe-Project.
2	Define the training level.	"Define training" on Start display, "Training Level" on sub window (Figure 6, manuscript)
3	Set the acceleration mode.	Set "20x" on sub window "ProcessStart - Start up" (Figure 6, manuscript)
4	Open the required GUIs.	"Mixing/Hydrolysis" on Start display (Figure 6, manuscript)
5	Check all pumps and motors for the mixing and hydrolysis unit. Start them if necessary.	Push "Start" on sub windows for motors and pumps (Figure 6, manuscript).
6	Set manually flow rates for flour, LF-enzyme, water and A- and B-starch as well as SF-enzyme added to the blender as calculated from the internal calculation sheet (not provided).	FIC 208: 1000 $kg \cdot h^{-1}$ FIC 022: 2000 $L \cdot h^{-1}$ FIC 1023-1: 2.6 $L \cdot h^{-1}$ FIC 002: 0.0 $L \cdot h^{-1}$ FIC 004: 0.0 $L \cdot h^{-1}$ FIC 1023-2: 3.0 $L \cdot h^{-1}$ Controller sub-window: "M"
7	Check set points of the controllers and start automatic control after you adjusted the rates manually.	FIC 208: 3500 $kg \cdot h^{-1}$ FIC 022: 7000 $L \cdot h^{-1}$ FIC 1023-1: 2.6 $L \cdot h^{-1}$ FIC 002: 0.0 $L \cdot h^{-1}$ FIC 004: 0.0 $L \cdot h^{-1}$ FIC 1023-2: 3.0 $L \cdot h^{-1}$ LIC 021: 35% Controller sub-window: "A"
8	Check set points of the controllers for the liquefaction unit and start automatic control.	LIC 023-3: 27.5 m^3 023-TIC 0201: 90 °C TIC 023: 60 °C Controller sub-window: "A"
9	Take a sample from the LF tank at least every 3 h. Record in an Excel-sheet the measured data for the LF tank.	Click "Sample" and choose "LF tank" Process time Dry mass pH (cf. Figure 7, manuscript: "Sample - LF tank")
10	Keep dry mass in the LF tank at 30% by adjusting controller set points for flour and starch mass/flow rate as well as water flow rate. (If necessary adjust the starch concentration of B-starch (A-starch) in the calculation sheet and adjust pump rates.)	FIC 208 FIC 022 FIC 002 FIC 004
11	Start the stirrer of the LF tank when 40% of the total volume is reached.	Push motor symbol above LF tank. Sub window: Motor LF tank "Start"

12	When the level controller starts the flow to the SF1 tank (P023.04.02), adjust the flow rate for sulfuric acid and SF enzyme. Start automatic control for SF enzyme.	pHI 023-6: 40% FIC 1023-2: 3.0 $L \cdot h^{-1}$ Controller sub window: "A"
13	Take a sample from the SF1 tank at least every 3 h. Record in an Excel-sheet the measured data for the SF1 tank.	Click "Sample" and choose "SF1 tank" Process time Dry mass pH (cf. Figure 7, manuscrpt: "Sample - SF tank 1")
14	Keep pH in the SF1 tank at 4.5–4.8 by adjusting the flow rate for sulfuric acid (P024.04).	pHI 023-6
15	Observe, operate and control the process to keep it stable. Take samples and adjust pump rates if necessary.	-
16	You can interrupt the process or use an extra acceleration if necessary.	On "Start display": "Accelerate process" or "Interrupt process"
17	Use on-line data to get an overview of the running process.	Push "History" and choose the desired on-line data.
18	Alarm messages inform you when process values deviates ±30% from their set points and when tanks reaches their maximum. Delete old alarm messages.	-
19	Start the stirrer of the SF1 tank when 40% of the total volume is reached.	Push motor symbol above SF1 tank. Sub window: Motor SF1 tank "Start"
20	Stop the start-up simulation after SF3 tank reaches 60 m^3. Save on-line data for process analysis. Switch off the OTS and exit the program.	Start display: "Stop process" Save on-line data "On/Off" "Exit"

(F—Flow; L—Level; T—Temperature; I—Indicator; C—Control; M—Motor; P—Pump; LF—Liquefaction; SF—Sacchrification. Each element in the right column is found on the GUI of the hydrolysis section (Figures 2, 6 and 7, manuscript)).