Simulating a Wine Minimodel

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Fermentation of sugars by yeast generates ethanol, the principal process in manufacture of wine. In a closed batch process the accumulation of ethanol eventually inhibits further microbial action and fermentation stops, even though there may be sugar remaining. The systems diagram in Figure 1 shows the main features of the wine system. On the left are the grapes with their sugars (tank shaped symbol on the left). In the middle are the yeast cells, which consume the sugars, releasing the by-product ethanol from their anaerobic metabolism. The hexagon shaped consumer symbol in the center represents the yeast. Within that symbol is the storage of functioning yeast biomass, from which there is a feedback (to the left) interacting and multiplying the intake, thus representing growth and reproduction. The production process is represented by the pointed-block symbol. A flow of ethanol is shown coming from the production symbol as by-product to the yeast production. The ethanol pathway goes into the ethanol storage (tank symbol) on the right. At the bottom is the stress symbol in which the ethanol interacts to destroy the yeast cells. The outflows of degraded heat energy are shown passing out of the system frame at the bottom (heat sink symbol).

Energy Systems Diagram of the Fermentation Minimodel with Equations

The energy systems diagrams automatically convert verbal models into equations, since each symbol has a mathematical equivalent. See recent book for this methodology (Odum and Odum, 2000). The rate equations that are implied by the model are included in Figure 1. The model was simulated earlier using BASIC (Beyers and Odum, 1993).

Rate equations constitute a model for computer simulation, after coefficients (k's in Figure 1) are calibrated. Values for calibration were assumed as follows: one liter of solution, 100 ml (milliliters) of grape sugars to ferment, a yeast population of one ml, production of new yeast at 2 ml/day, a resting metabolism-loss of yeast of 0.5 ml/day, an ethanol production of 0.5 ml/day, a stress removal of yeast of 2 ml/day when the ethanol storage is 10. Loss of grapes and ethanol storages due to dispersal and other factors was made negligible.

Simulation with General System Symbols

The model was simulated with the program EXTEND for which we have object oriented blocks preprogrammed for the energy system symbols.

See Figure 2a. With these blocks calibration is done by typing the storages and flows into dialog boxes of the four symbols used. These dialog boxes after calibration are shown in Figure 2b-e.

Figure 3 is the simulation with these values. The grapes-sugar decreases, yeast grows quickly, and ethanol accumulates. The yeast declines as the sugar gets less and the ethanol eliminates active cells. In this run, fermentation stops with considerable sugar remaining unfermented.

If the pathway from ethanol stressing the yeast is eliminated, and the model is run again, the yeast without inhibition uses up the sugar and then declines for lack of an energy source.

Simulation with Pictorial Icon Blocks

The model was also simulated with specialized blocks, which have picture-icons and calibrations programmed within the blocks, out of sight from the user. Four special icons: Grapes, Yeast, Ethanol, and Inhibition, were made from the general symbols by setting the calibration coefficients within the script of the program. These picture symbols are connected to form the same system in Figure 4 as the general system version in Figure 3. The dialog boxes only have one item each, that the user can easily change (initial storages, and stress factor for the ethanol). Figure 5 is the simulation result, which is the same as the one with the general systems symbols.

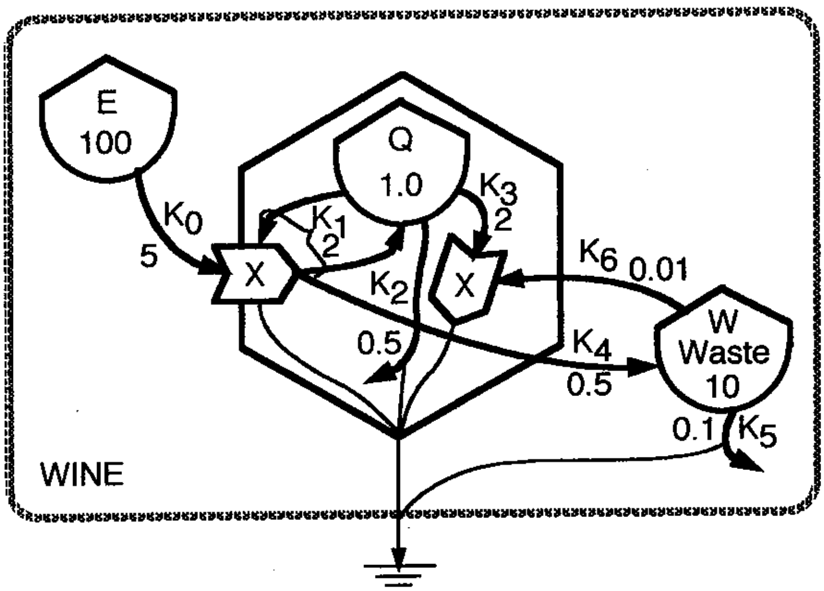
Although this model has grapes, yeast and alcohol, the design is recurring in other situations where by-products accumulate and inhibit the main conversion process. This model might apply on the large scale of human society if its waste products accumulate enough to inhibit the production of humanity.

Simulation Procedure

1. Load EXTEND
2. Use menu to open "WINE" (which automatically loads WINELIB library.
3. Use menu to RUN the program; then make "What if?" changes.
4. Repeat with the general symbols version WINEGS.

Beyers, R.J. and H.T. Odum. 1993. Ecological Microcosms. Springer-Verlag, NY, 545 pp.

Odum, H.T. and E.C. Odum. 2000. Modeling for All Scales, an Introduction to Simulation. Academic Press, San Diego, CA, 458 pp.



$$\dot{E} = -K_0EQ$$

$$\dot{Q} = K_1EQ - K_2Q - K_3WQ$$

$$\dot{W} = K_4EQ - K_5W - K_6EQ$$

Figure 1. Minimodel of wine production (WINE) drawn with energy systems symbols and resulting change equations.

Fig. 2(a)

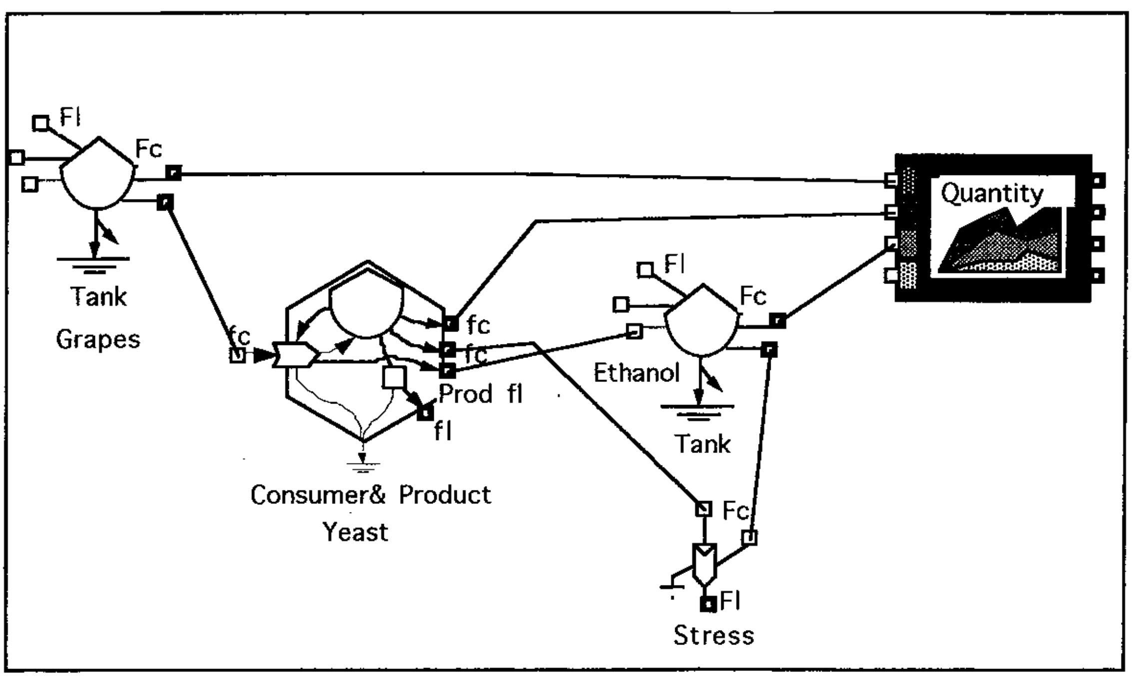


Figure 2. WINEGS model with general systems blocks connected for simulation with EXTEND. (a) Screen view; (b) dialog box of storage tank with grapes; (c) dialog box for yeast consumer unit; (d) dialog box for the stress block; (e) dialog box for the ethanol storage.

Fig. 2(b)

Enter Calibration values:

When Storage is:	1.000e+02
Depreciation flow is:	0.01

Enter Starting Values:

Starting Storage is:	100
Starting Transformity is:	10000

OK | Cancel | Help

Fig. 2(c)

Enter calibration values:

Quantity of assets:	1
Productive contribution to assets	2
Production byproduct outflow	0.5
Depreciation of assets	0.5
Materials released by depreciation	0.05
Left input quantity	100
Left input flow	5
Enter starting Quantity:	0.1

OK | Cancel | Help

Fig. 2(d)

For the calibration condition:

Enter the flow from above :	2
when the quantity there is :	1
Enter the flow from right (stress):	0.01
when the quantity there is:	10
For the two quantities used in calibration (above), enter the product flow:	3

OK | Cancel | Help

Fig. 2(e)

Enter Calibration values:

When Storage is:	1.000e+01
Depreciation flow is:	0.1

Enter Starting Values:

Starting Storage is:	0.1
Starting Transformity is:	10000

OK | Cancel | Help

Fig. 3(a)

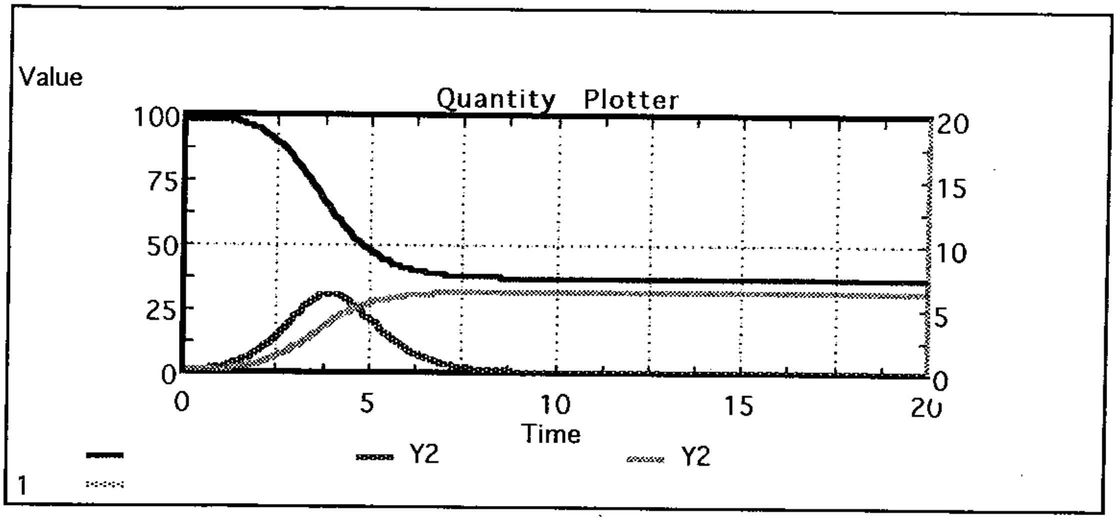


Fig. 3(b)

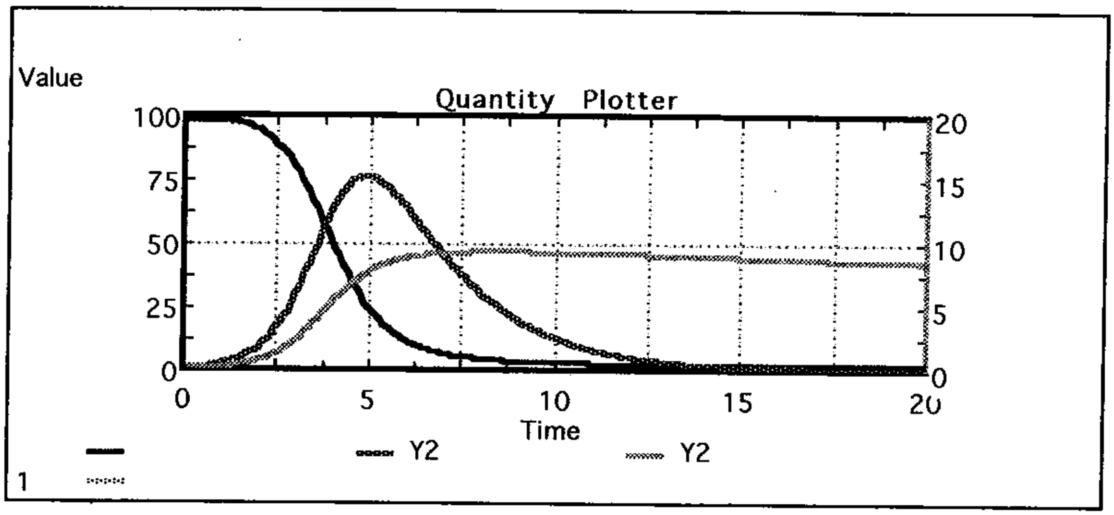


Figure 3. Results of simulating the models in Figures 2 and 4. (a) As calibrated; (b) with stress disconnected.

Ferment

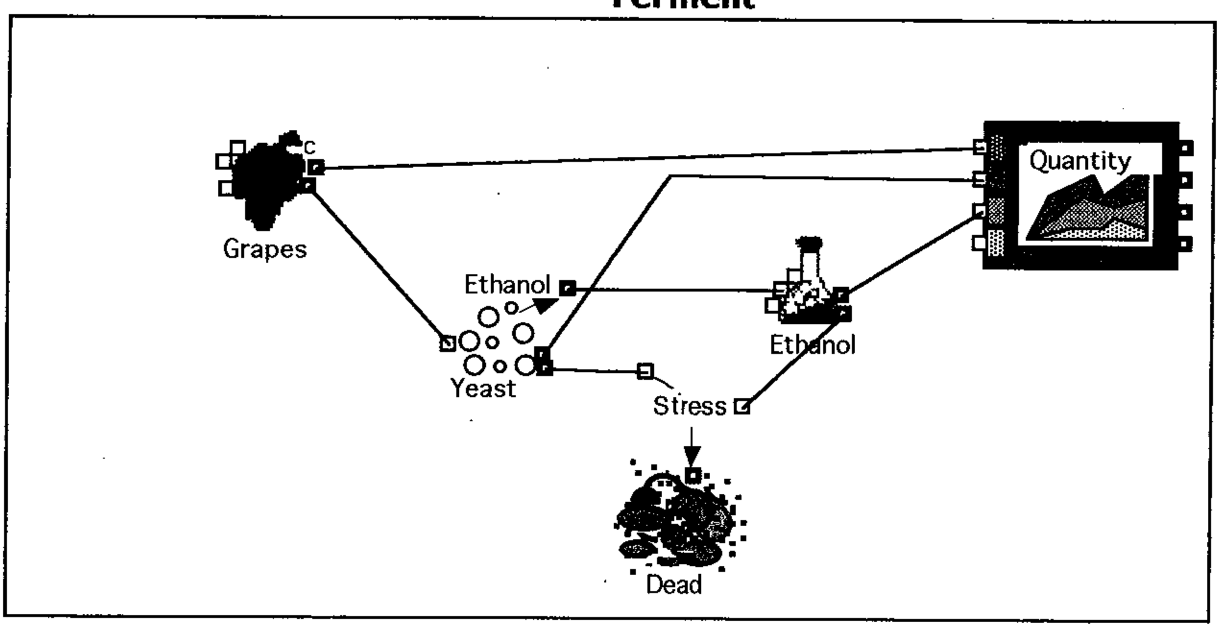


Figure 4. Fermentation model with picture icon blocks.