VISIMIX TURBULENT.
EVALUATION OF PROCESS DURATION IN A GAS-LIQUID REACTOR.

Problem description:

A chain of chemical reactions, including oxidation reaction is carried out in a water phase in a pilot reactor. The oxygen comes from the air injected underneath the impeller.

Gas-liquid mass transfer is the limiting stage of the process, since the reactions in the liquid phase are assumed to be fast.

Oxygen from the air is absorbed by the system and participates in the reaction. In the pilot vessel, the reaction requires 1 hour.

Initial data

The pilot reactor is a baffled tank with elliptical bottom with a total volume of 60 liter, single stage disk turbine impeller (Figures 9-1--9-3). The reaction is carried out in a water solution at room temperature. The system has no special surfactants. Gas flow rate is 10 cub. m/hour.

The process must be scaled up to the available production-scale reactor. Its parameters are as shown in Figures 9-11--9-14. The air flow rate in the production-scale system can vary in the range 100-300 cub. m /hour.

The task is to evaluate the time needed to complete this reaction in the industrial reactor.

The Solution:

This problem can be easily solved with VisiMix. The required value can be obtained using the simple formula:

$$M = G\ \tau\,/\,V = G^{specific}\tau\,,$$

where

M is specific gas consumption during the entire process, Kg/l;
G is gas mass transfer rate, Kg/hour;
$G^{specific} = G/V$ is specific gas mass transfer rate, Kg/(hour·l);
τ is process duration, hours, and
V is the media volume in the reactor, l

Gas mass transfer rate, G is calculated by VisiMix directly. Therefore, you will first calculate gas mass transfer rate, G_{pilot} for the pilot reactor. Then you will check specific oxygen consumption, M_{pilot} for the pilot process, i.e. how much oxygen per liter is absorbed in the pilot reactor during the entire process, using the formula adduced above.

Then you'll calculate gas mass transfer rate, $G_{production}$ for the production reactor, and divide it by the media volume to obtain specific gas mass transfer rate, $G_{production}^{specific}$ for the production reactor.

Now you will be able to estimate the duration of the production-scale process, $\tau_{production}$. Since gas-liquid mass transfer is the limiting factor for this reaction, the process duration is the time required for achieving the same value for specific oxygen consumption obtained for the pilot process. Thus,

$$\tau_{production} = M_{pilot} / G_{production}^{specific}$$

To perform the calculations, you must create two VisiMix projects: one for the pilot reactor, and another for the available production-scale reactor. Let us first enter parameters of the pilot reactor. Select **Project - New** in the VisiMix main menu, and provide a name for the pilot project, for example, **gaspilot.vsm**. In the graphical tanks selection, select your pilot tank (unjacketed tank with elliptical bottom) and enter its parameters in the input table that appears (Figure 9-1).
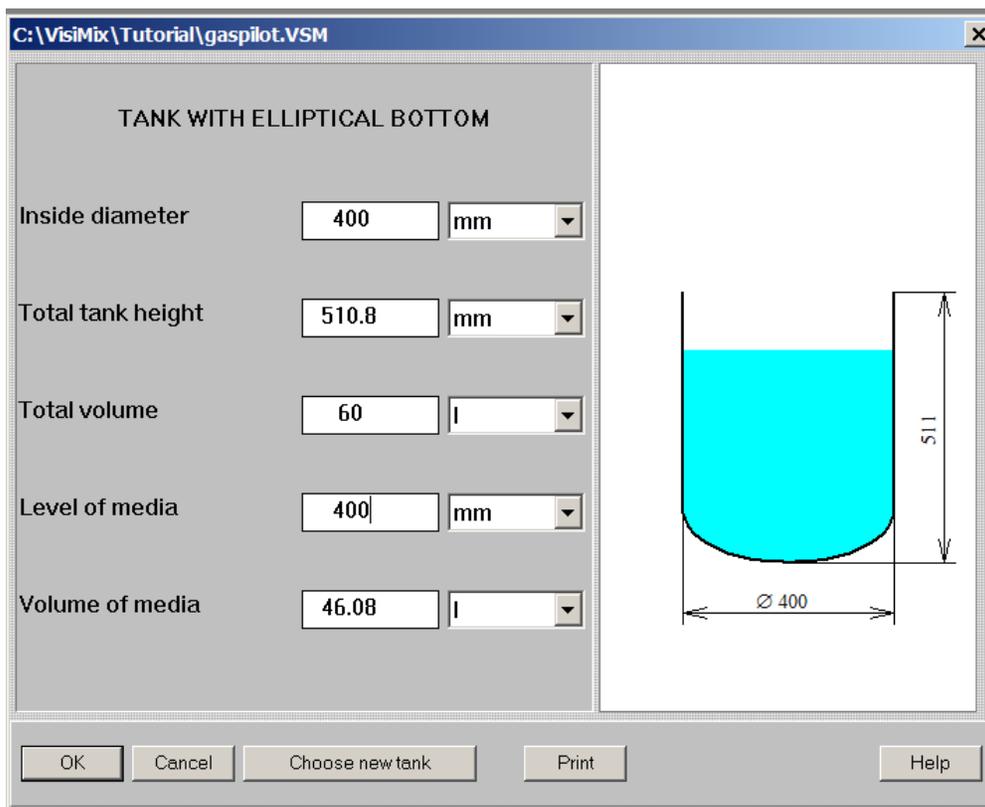

Figure 9-1. Entering tank data (pilot).

Click **OK**, select baffle type (Flat baffle -1 in your case), and enter baffle parameters as shown in Figure 9-2.
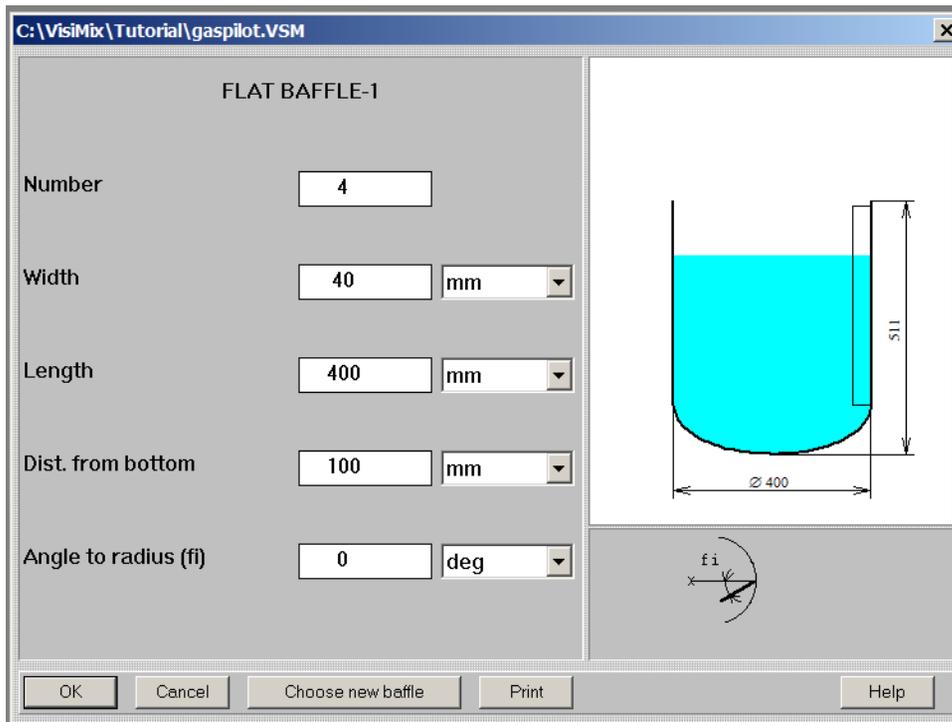
Figure 9-2. Entering baffle data (pilot).

Now click **OK**, and select the impeller type (single stage disk turbine), then supply impeller parameters as shown in Figure 9-3.
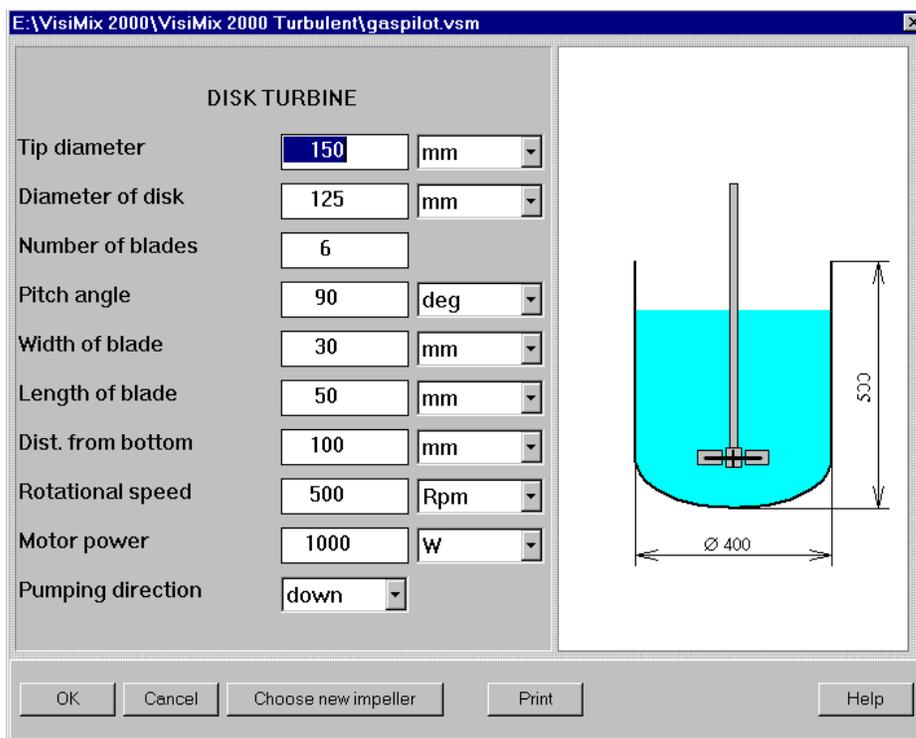

Figure 9-3. Entering impeller data (pilot).

Click OK, and enter average properties for the media (water) as shown in Figures 9-4a and 9-4b.
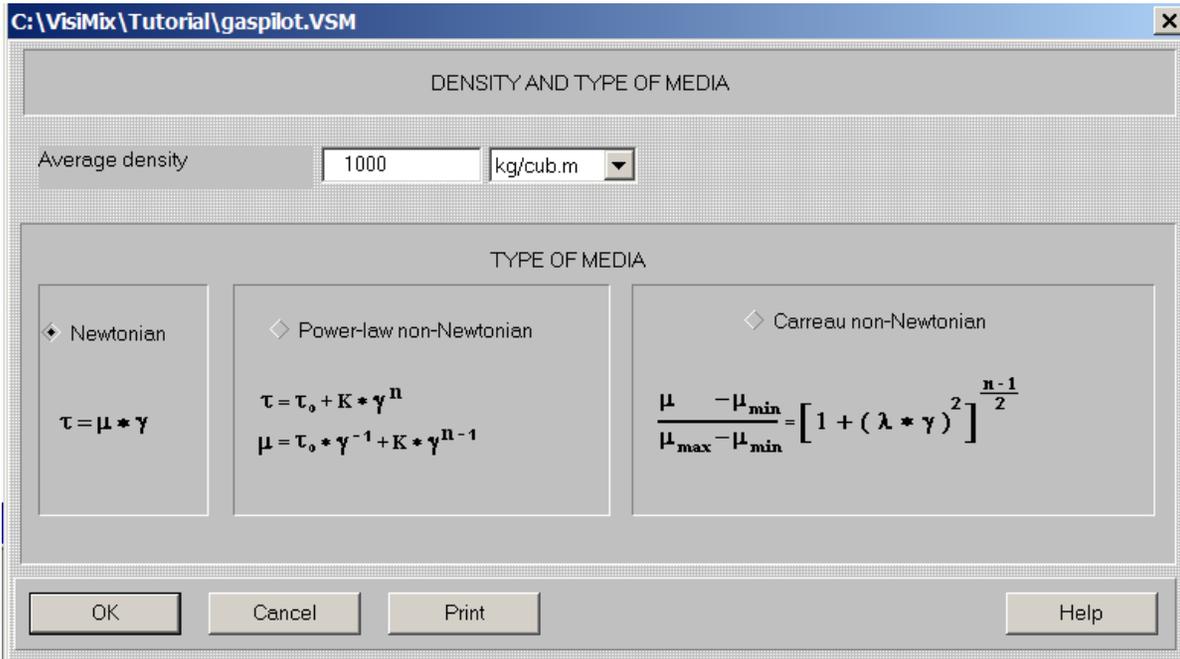
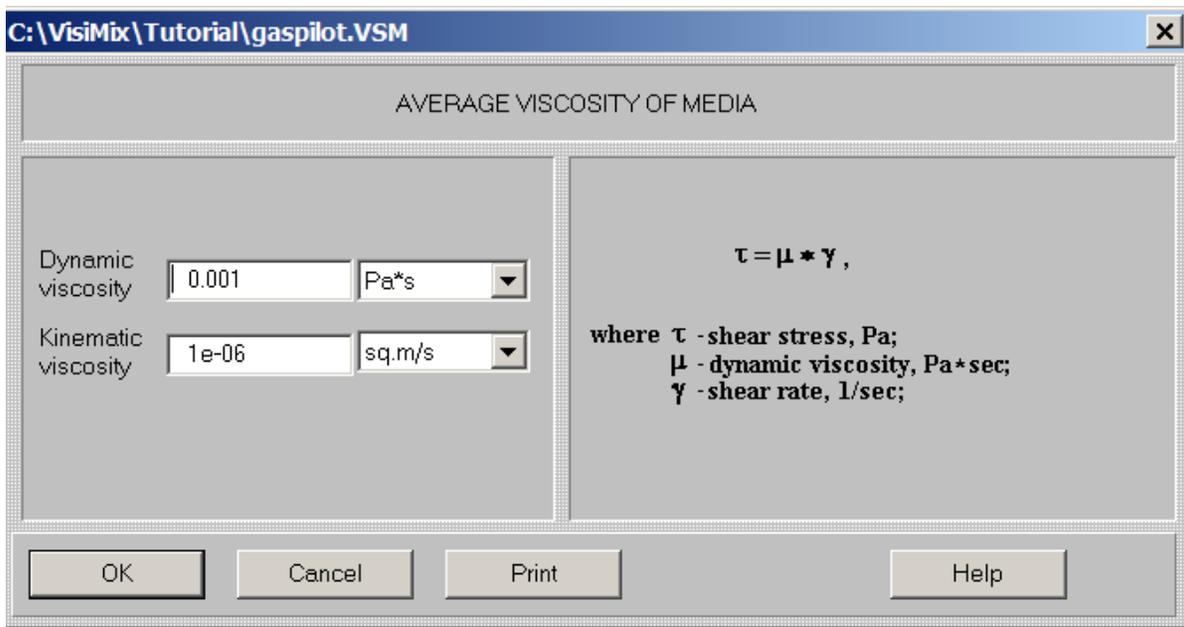*Figure 9-4a. Entering density and type of media.*

Figure 9-4b. Entering viscosity of media

You have now entered all basic data for your pilot reactor, and its diagram corresponding to the data you have entered appears on the screen (Figure 9-5).
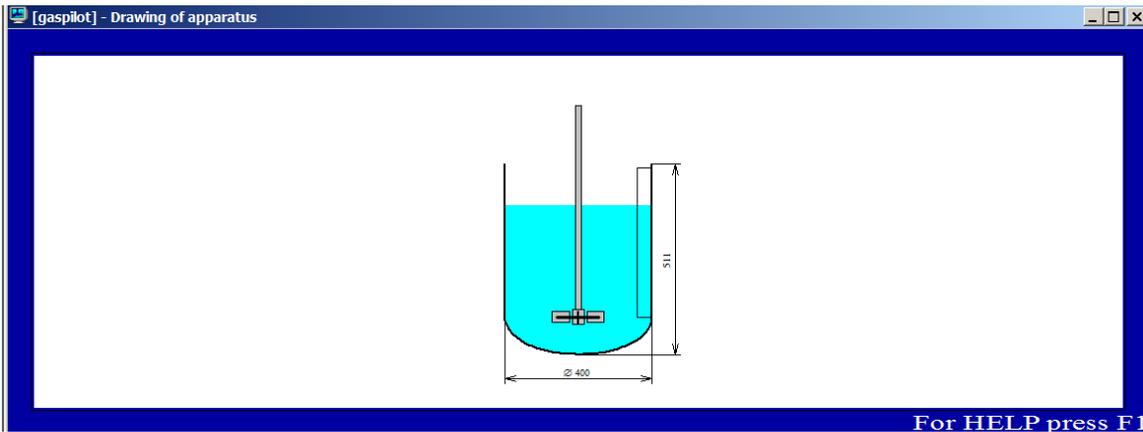
Figure 9-5. The diagram of the pilot mixing system

Let us now calculate gas mass transfer rate for the pilot reactor. In the main VisiMix menu, select **Calculate**, **Gas dispersion**, then **Gas mass transfer rate, kg per hour** (Figure 9-6).
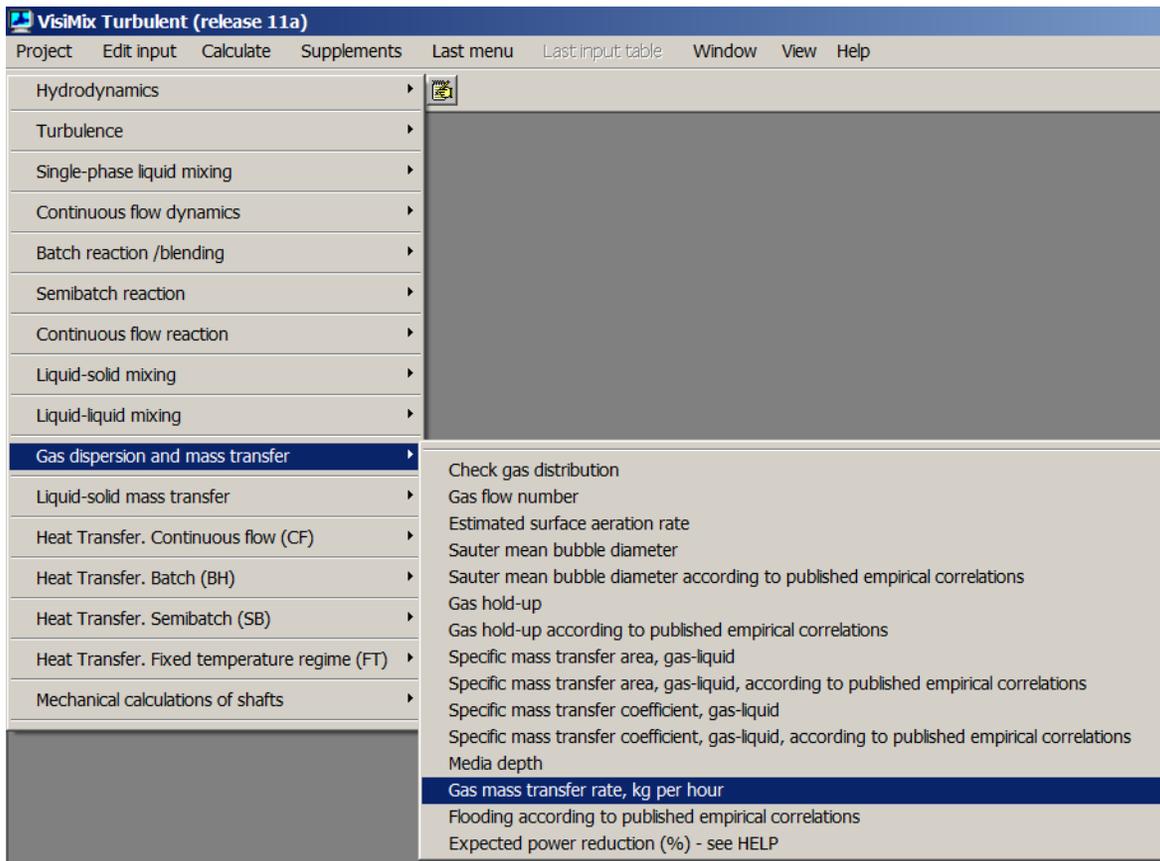

Figure 9-6. Selecting a parameter for calculation.

To calculate **Gas mass transfer rate**, additional data is needed. VisiMix requests this data by invoking the appropriate input tables.

The first table is GAS DIFFUSIVITY input table appears. Enter the diffusivity value for oxygen in water at 20°C. Data can be taken from the appropriate table in the Help section (Figure 9-7).

Figure 9-7. Entering gas diffusivity.

Click **OK**, and GAS SOLUBILITY input table appears. Enter the solubility value in normal conditions for contact with air (Figure 9-8a). You shall enter "0" as **Mass gas concentration in solution** since your reactions are fast, and the process rate is limited by gas-liquid mass transfer.

Figure 9-8a. Entering gas solubility

SURFACE TENSION is entered from reference data (you may click on Help to invoke the appropriate reference table). You select the value of surface tension given for pure water (Figure 9-8b), since there are no surfactants in your system.

Figure 9-8b. Entering surface tension

Click OK, and GAS DISPERSION BASIC DATA. Supply the requested parameters as shown in Figure 9-9. **Volume flow rate** for your process is known, and the **Superficial gas velocity** is calculated by the program and entered automatically.
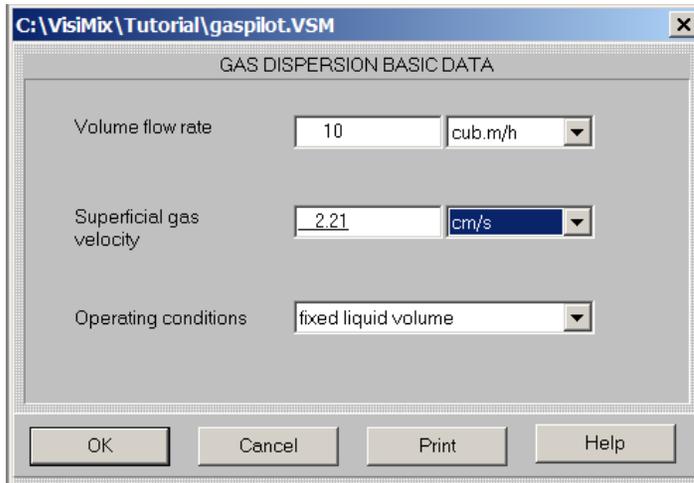

Figure 9-9. Entering gas dispersion basic data (pilot).

When this table is completed, VisiMix starts calculations, and the desired **Gas mass transfer rate** value appears on the screen (Figure 9-10).

Figure 9-10. Gas mass transfer rate (pilot).

Now let us determine oxygen consumption per liter during the entire process, M_{pilot}. Gas mass transfer rate must be multiplied by the process duration and divided by the media volume:

0.246 x 1 hour / 46.08 = 0.0053 kg/l (5.3 g/l)

Let us now save the project and create another project for your production-scale reactor. Since some initial data for the production process is already stored in VisiMix, you will create your production project from the pilot one using **Save as** option. Let us call the second project gasproduction.vsm, and enter the data for the production reactor by modifying data in the appropriate input tables (Figures 9-11 -- 9-13). All input tables are accessible from the **Edit input** option in the main menu.
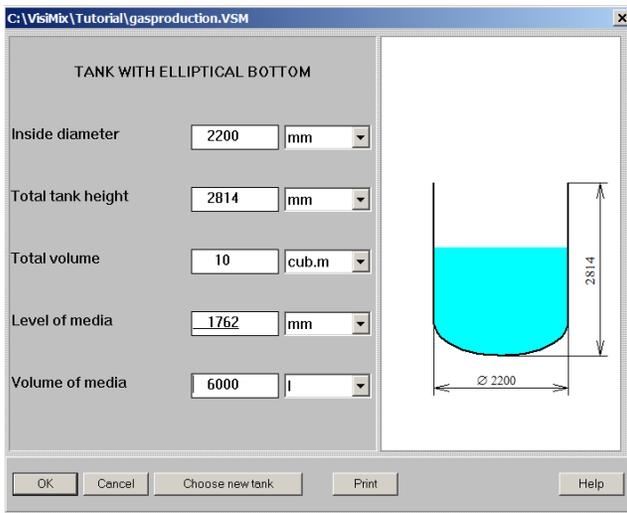
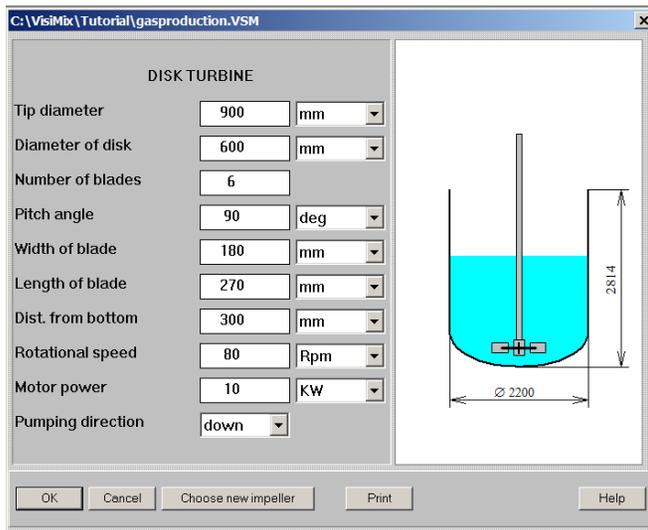*Figure 9-11. Entering tank data (production scale).*

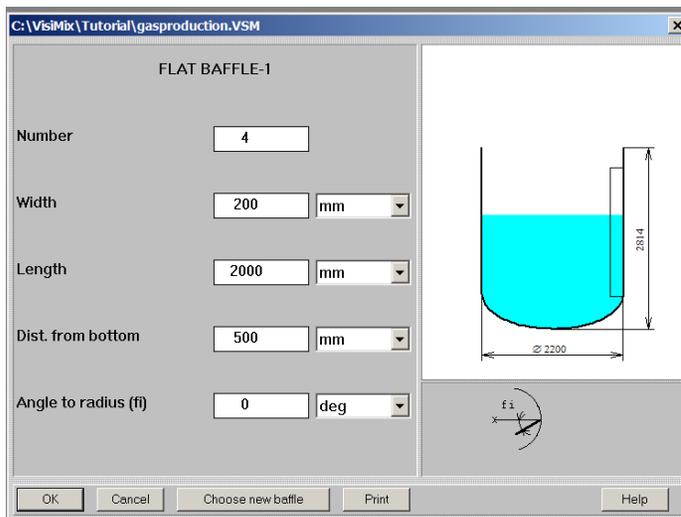*Figure 9-12. Entering impeller data (production scale)*

Figure 9-13. Entering baffle data (production scale).

Average properties of the media, gas solubility and gas diffusivity are naturally the same as in the pilot process. Let us now enter **Volume flow rate** (input table GAS DISPERSION BASIC DATA), starting from the lower limit of the prescribed range of values, i.e. 100 cub. m per hour (Figure 9-14).
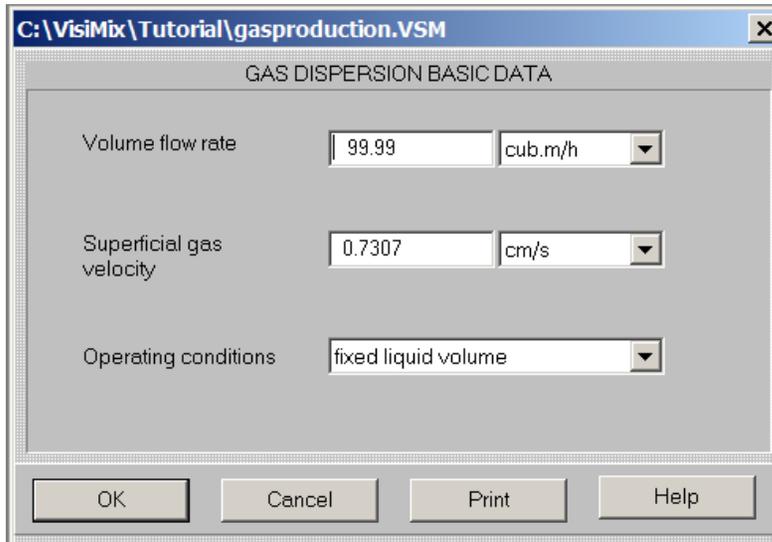

Figure 9-14. Entering gas dispersion basic data (production scale)

In order to estimate the process duration in the production reactor, let us start from calculation of gas mass transfer rate for the production reactor. The result is shown in Figure 9-15.

Figure 9-15. Gas mass transfer rate (production scale)

As described above, let us divide it by the media volume in the production reactor to obtain specific gas mass transfer rate value, $G_{production}^{specific}$:

(5.82 kg/hour) / (6000 l) = 0.00097 kg/(hour·l), or 0.97 g/(hour·l)

The specific oxygen consumption value, M_{pilot} obtained earlier for the pilot reactor is 5.3 g/l. Thus, the desired value for process duration in the production reactor can be obtained as follows:

5.3 / 0.97 = 5.46 (hours)

Let us now check if it is possible to reduce this time by increasing volume flow rate of air injected underneath the impeller.

Select **Edit input, Properties & regime, Gas dispersion basic data**, and enter the maximum allowable value for gas flow rate, which is 300 cub. m /hour. Click OK to confirm your input. The modified output table shown in Figure 9-15 immediately appears on the screen (Figure 9-16).

[gasproduction] - Gas mass transfer rate, kg per hour		_ □ ×
GAS MASS TRANSFER RATE, KG PER HOUR		
Parameter name	Units	Value
Gas mass transfer rate, kg per hour		18.0

For HELP press F1

Figure 9-16. Gas mass transfer rate (production scale), modified.

After repeating the calculations of the process duration, you'll obtain 1.77 hours. You have thus succeeded in reducing the process duration by increasing the gas volume flow rate, though the process duration is still considerably longer than in the pilot reactor.