VISIMIX TURBULENT.
LIQUID - LIQUID MIXING. DROP SIZE. SCALING – UP.

In mixing of immiscible liquids, two rivaling processes of break-up and coalescence of drops occur simultaneously. The intensity of both processes and, therefore, the results of emulsification are determined by local mixing intensity (shear rate, specific power, etc.) which, in turn, depends on characteristics of tank and impeller, and on the physical properties of the initial fluids.

VisiMix simulates the formation of the emulsion, determines if complete emulsification is achieved, calculates mean drop size, specific mass transfer area, mixing time, and other process parameters important for emulsification, liquid extraction, multiphase chemical reactions etc.

This example shows how to successfully perform scaling-up of a liquid-liquid extraction process.

Problem description:

A liquid-liquid extraction process is carried out in a pilot reactor. In the pilot process, emulsification is satisfactory, and stabilization time for achieving the balance between break-up and coalescence is small (considerably less than 10 min). This process must be scaled up so that the same or similar emulsification quality is achieved in an industrial reactor, either already available, or modified by accessible means.

In industrial and pilot reactors, the following scaling-up parameters must be identical:

- Stabilization time for achieving the balance between break-up and coalescence (considerably less than 10 min);
- Specific mass transfer area.

The task is to determine these parameters for both pilot and production-scale reactors in order to make sure that the operation conditions in the production-scale reactor are close to those in the pilot unit.

Initial data

Pilot reactor:

Tank (with elliptical bottom):
Inside diameter = 300 mm;
Total volume = 30 liters;
Volume of media = 20 liters.

Baffle (flat type, attached at a distance from the wall)
Number = 4;
Width = 30 mm;
Length = 250 mm;
Distance from bottom = 75 mm;
Distance from wall = 5 mm;

Angle to radius = 0 deg.

Impeller (disc turbine)
Tip diameter = 100 mm;
Diameter of disc = 75mm;
Number of blades = 6;
Pitch angle = 90deg;
Width of blade = 20 mm;
Length of blade = 25 mm;
Distance from bottom = 100 mm;
RPM = 350;
Power of drive = 100 W;

Production-scale reactor (basic variant)

Tank (with elliptical bottom):
Inside diameter = 1800 mm;
Total volume = 6m^3;
Volume of media = 5m^3.

Baffle (double tubular type)
Number = 1;
Width (tube diameter) = 100 mm;
Length = 1300 mm;
Distance from bottom = 450 mm;
Distance from wall = 100 mm;
Angle to radius = 0 degrees

Impeller (Glass lined impeller-1)
Tip diameter = 800 mm;
Number of blades = 3;
Width of blade = 80 mm;
Distance from bottom = 500 mm;
RPM = 100;
Power of drive = 10 kW;

Media properties

The media is a pure oil - water system without significant admixtures with the
interfacial surface tension = 0.03 N/m; its average properties are close to those of pure
service water.

Continuous phase (water) properties:
     Density = 1000 kg/cub. m;
     Dynamic viscosity = 0.001 Pa*s;
Disperse phase (pure oil) properties:
     Volume fraction = 0.15;
     Density = 940 kg/cub. m;
     Dynamic viscosity = 0.03 Pa*s;

The Solution:

The general sequence of operations is as described above in other examples of this **Tutorial**.

For the given case, you must calculate and compare 2 parameters: stabilization time for achieving the balance between break-up and coalescence, and specific mass transfer area.

The first can be obtained from the graph **KINETICS OF DROP BREAK-UP** in the **Liquid-Liquid Mixing** option of **Calculate**, and the second can be obtained from this option directly.

Before proceeding to calculations, you must enter initial data for both pilot and production-scale reactors. Start with the pilot simulation, and then consider the available production-scale reactor, changing its parameters if necessary.

Following the standard VisiMix procedure, start a new project for your pilot reactor.

Select **Project,** then **New,** then enter the name for your project (**Scale-up-pilot.vsm** in this example, as shown in Figure 3-1).
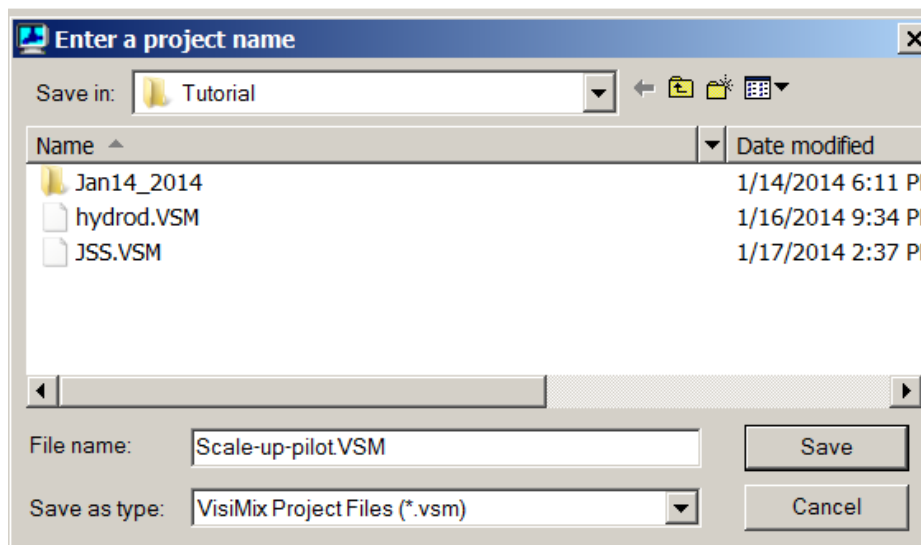
Figure 3-1. Starting a new project.

Click **Save**, and select your tank in the **Tank types** selection that appears. The tank you have selected (elliptical bottom without heat transfer device) will appear in the **Current choice** window on the right (Figure 3-2). Click **OK** to confirm your choice.
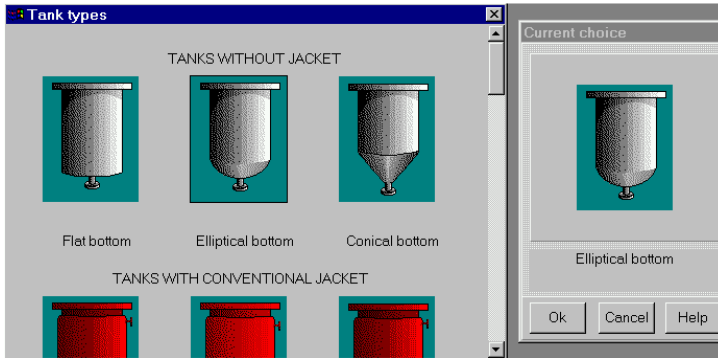
Figure 3-2.   VisiMix graphic tanks selection.

Now you will be requested to enter basic initial data for your project. After you confirm your tank choice, TANK WITH ELLIPTICAL BOTTOM input table with the selected tank diagram appears. Supply the internal dimensions of your tank. Enter **Inside diameter**, **Total volume** and **Volume of media,** and **Total tank height** and **Level of media** will be calculated by the program and entered automatically (Figure 3-3).
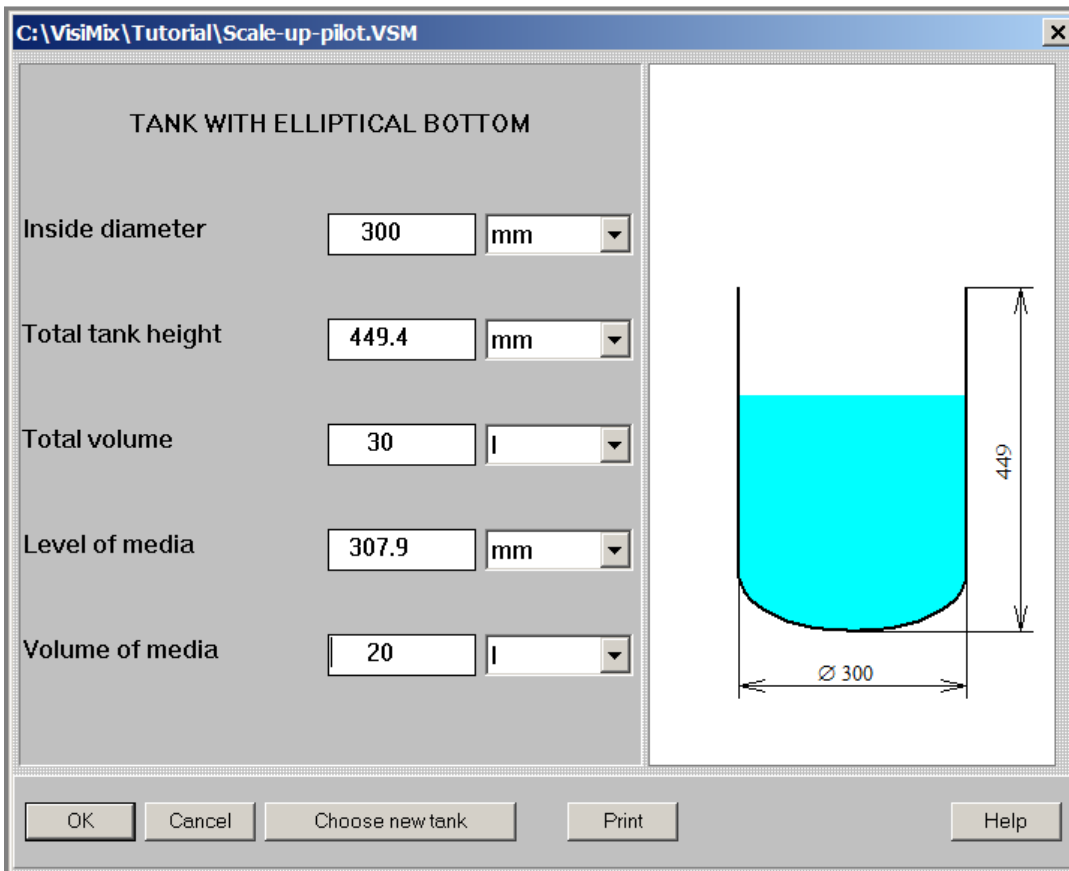

Figure 3-3. Entering pilot tank data.

After the table has been completed, click anywhere on the field of the window, and the tank diagram on the screen will change to reflect your input. Click **OK** to confirm your input.

The **Baffle types** menu will now appear. Click on the diagram of the selected baffle (Flat baffle – 2 in your case), and it will appear in the **Current choice** window on the right (Figure 3-4). Click **OK** to confirm your choice.
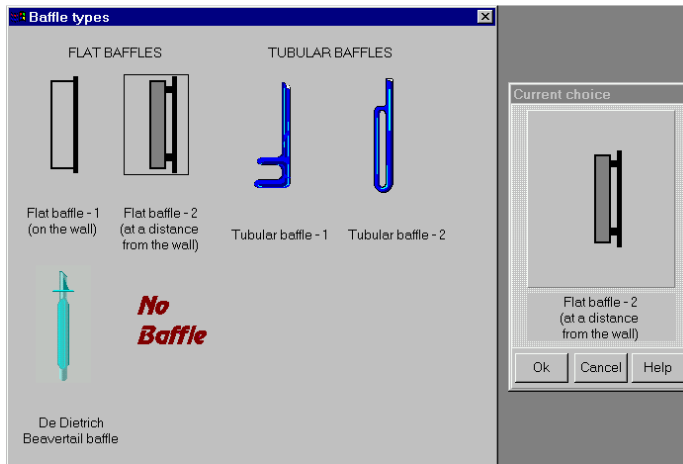

Figure 3-4. Selecting a baffle for the pilot reactor.

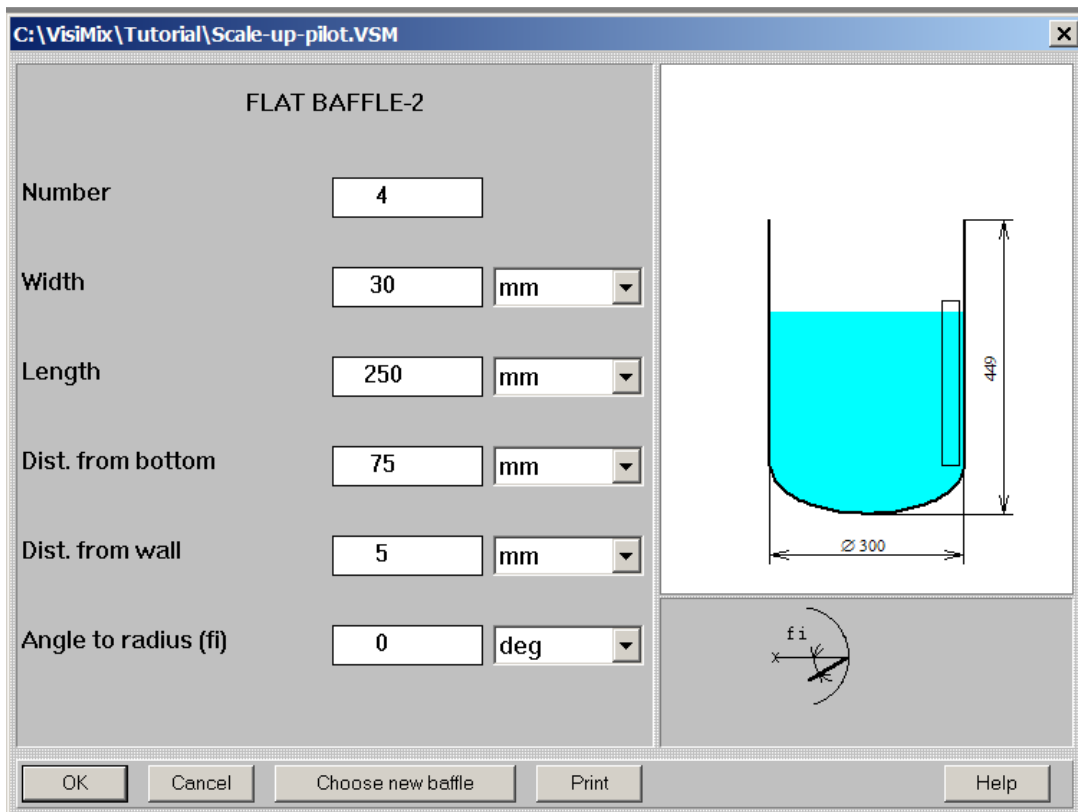Enter parameters of your baffle in the table that appears (Figure 3-5).

Figure 3-5. Entering baffle data for pilot reactor.

Now select your impeller in the **Impeller types** menu that appears (Figure 3-6). The **single** option for your single-stage mixing system is already selected (by default) in the **Current choice** window.
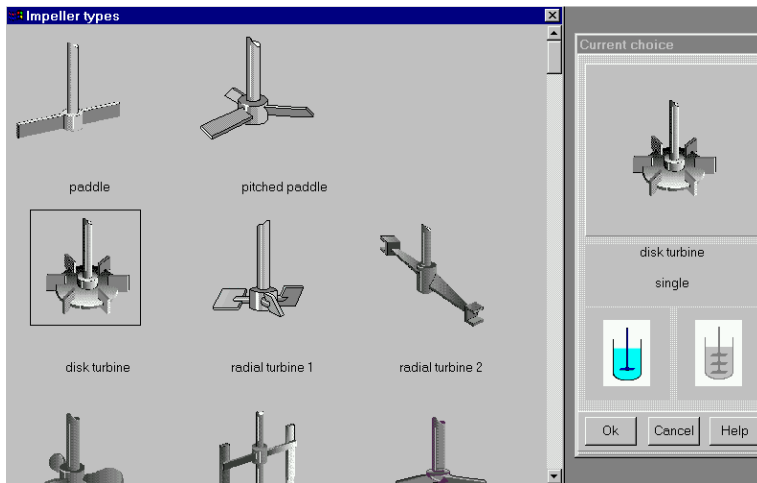
Figure 3-6. Selecting impeller for pilot reactor.

Enter impeller parameters in the input table that appears (Figure 3-7), then click anywhere in the field of the window, and the disc turbine diagram on the screen will change to reflect your input. Click **OK** to confirm your input.
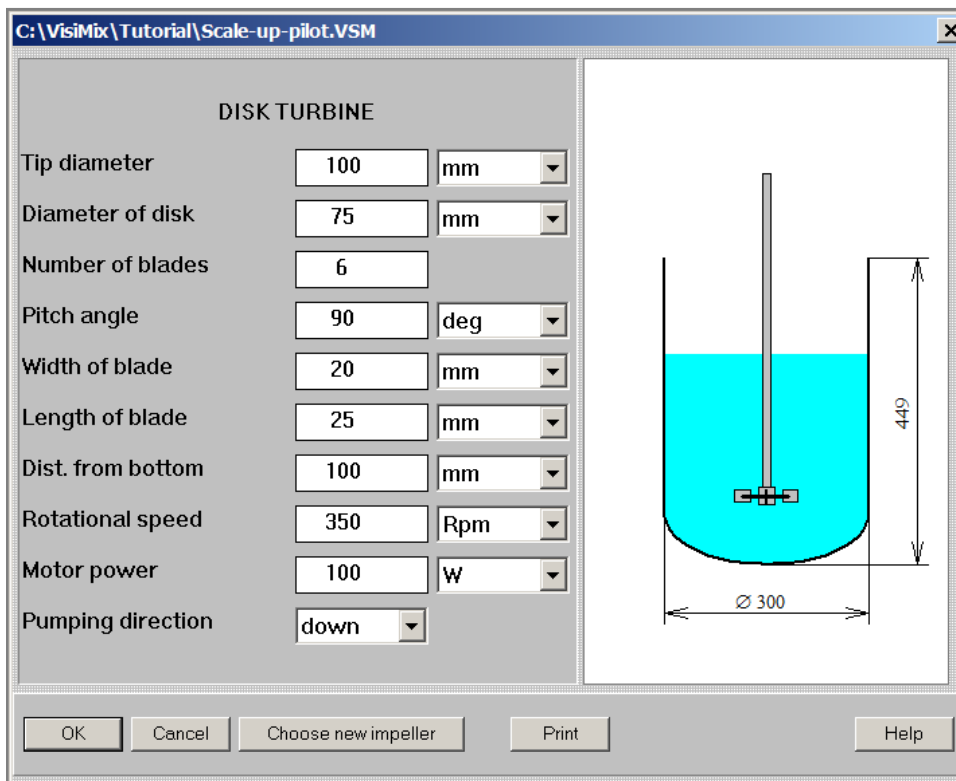

Figure 3-7. Entering impeller data for pilot reactor.

Now it is necessary to define average properties of media. At first you will be requested to fill out the DENSITY AND TYPE OF MEDIA input table (Figure 3-8a) and then the AVERAGE VISCOSITY OF MEDIA (Figure 3-8b). Since the properties of the media are close to those of pure service water, enter the properties of water as the first approximation.
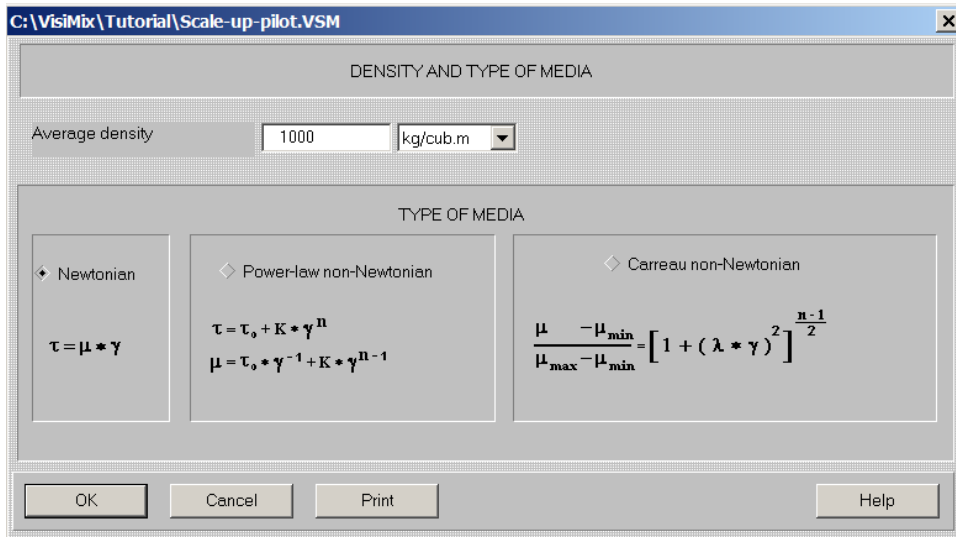
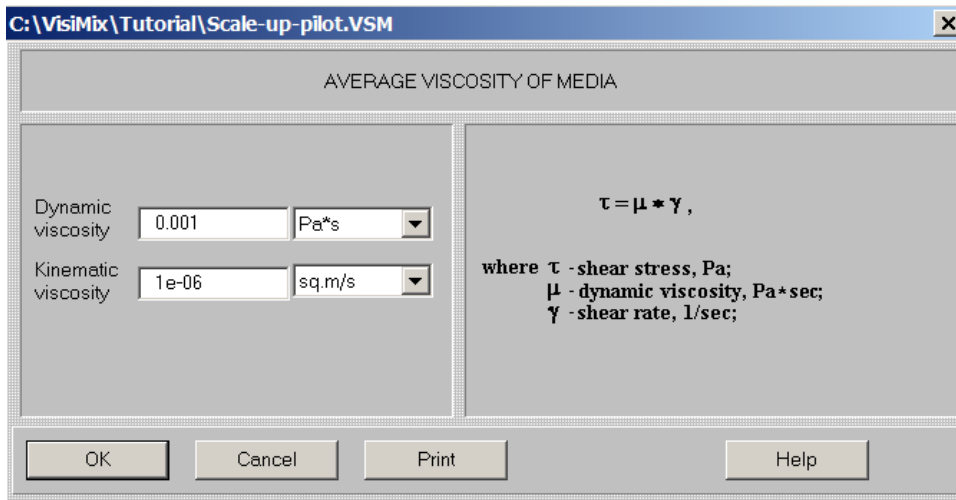**Figure 3-8a. Entering density and type of media.**

Figure 3-8b. Entering average viscosity of media.

After you have entered basic data for your pilot reactor, its diagram appears (Figure 3-9). From now on, you will be asked to enter only the data required for solving your particular problem selected in the **Calculate** option.
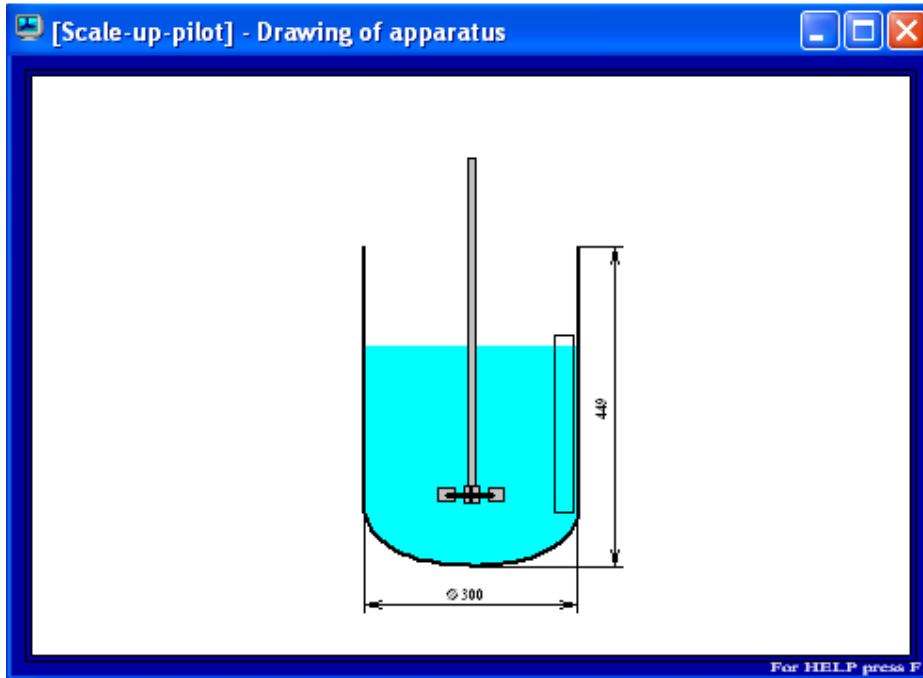
Figure 3-9. Tank diagram.

We recommend closing this window before proceeding to calculations.

To proceed to calculations, select **Calculate** in the main menu and click on **Liquid - liquid mixing**, then on **KINETICS OF DROP BREAK-UP.** Since additional data is required for calculations, you will be asked to complete PROPERTIES OF CONTINUOUS AND DISPERSE LIQUID PHASES input table (Figure 3-10).

Figure 3-10. Properties of continuous and disperse liquid phases.

Based on this data, VisiMix re-calculates the average properties of the media. If these calculated values do not correspond to the data entered earlier, you will receive a message shown in Figure 3-11.
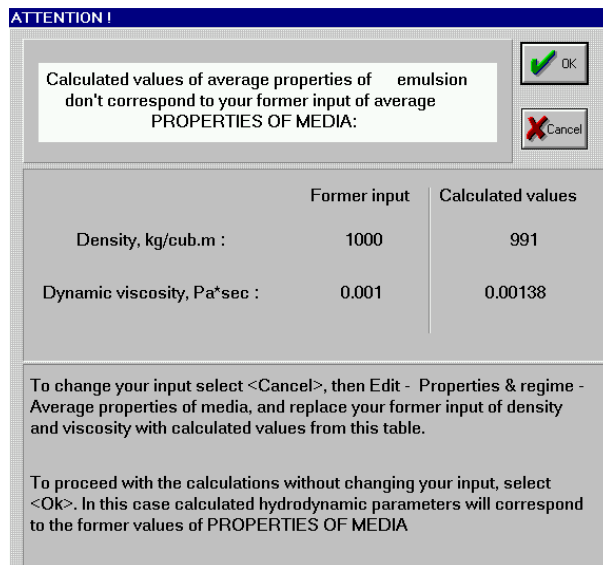

Figure 3-11. A message warning of the discrepancy between entered and calculated average media properties.

Let's follow VisiMix recommendations and correct the data entered in the tables corresponding to AVERAGE PROPERTIES OF MEDIA: DENSITY AND TYPE OF MEDIA (Figure 3-8a) and PARAMETERS OF RHEOLOGY (Figure 3-8b). Click **Cancel,** and the message shown in Figure 3-12 will appear.
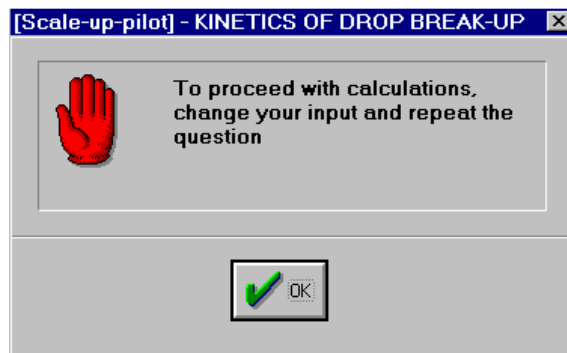

Figure 3-12. The message recommending to adjust input data.

Click **OK** and select **Edit input, Properties & regime, Average properties of media** and firstly **Density and type of media** and then **Parameters of rheology**. Replace your former input with recalculated data as shown in Figures 3-13a and 3-13b.
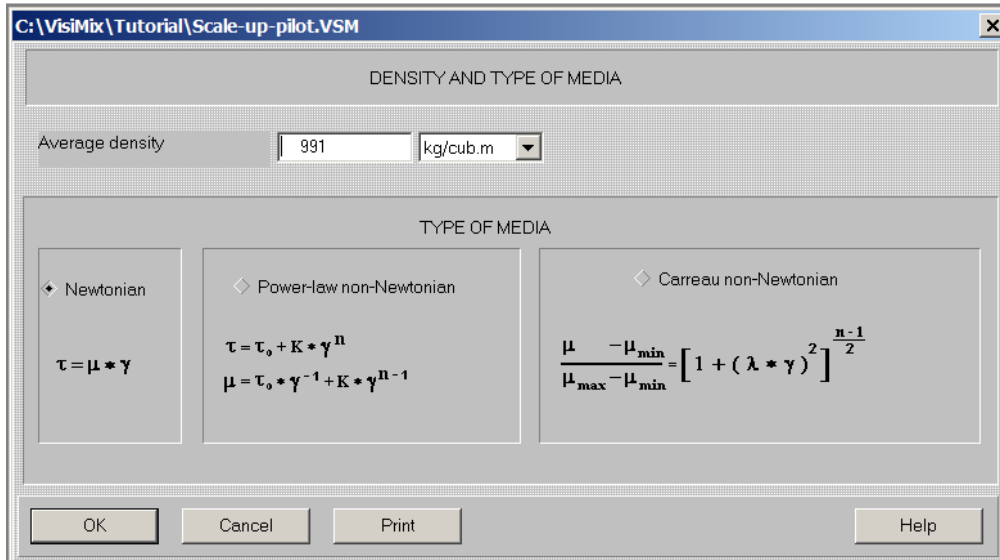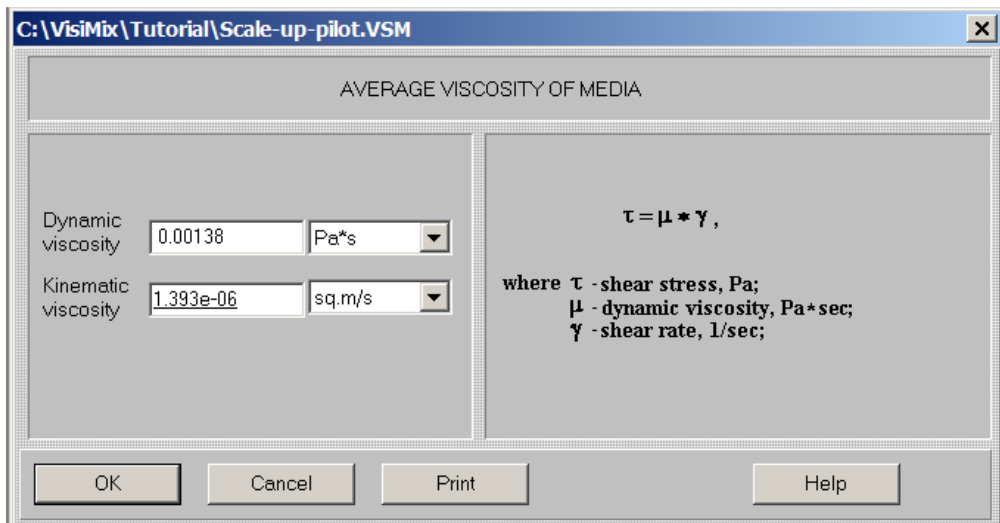
Figure 3-13a. Entering adjusted density.

The dialog shows:

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DENSITY AND TYPE OF MEDIA

Average density: 991 kg/cub.m

TYPE OF MEDIA

- Newtonian
$$\tau = \mu * \gamma$$

- Power-law non-Newtonian
$$\tau = \tau_o + K * \gamma^n$$
$$\mu = \tau_o * \gamma^{-1} + K * \gamma^{n-1}$$

- Carreau non-Newtonian
$$\frac{\mu - \mu_{min}}{\mu_{max} - \mu_{min}} = \left[1 + (\lambda * \gamma)^2 \right]^{\frac{n-1}{2}}$$

OK   Cancel   Print   Help

Figure 3-13b. Entering adjusted viscosity.

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AVERAGE VISCOSITY OF MEDIA

Dynamic viscosity: 0.00138 Pa*s

Kinematic viscosity: 1.393e-06 sq.m/s

$$\tau = \mu * \gamma,$$

where τ - shear stress, Pa;
μ - dynamic viscosity, Pa*sec;
γ - shear rate, 1/sec;

OK   Cancel   Print   Help

By now, you have entered all the required process and equipment parameters. Click **OK,** and select **Last menu** - **Kinetics of drop break-up.** In a very short time, all the required calculations will be finished, and a graph of **Kinetics of drop break-up** will appear (Figure 3-14). Click on **Start** to start the simulation, and you will see that stabilization time value is about 2 min. You have thus determined the first of the two scaling-up parameters for pilot reactor.
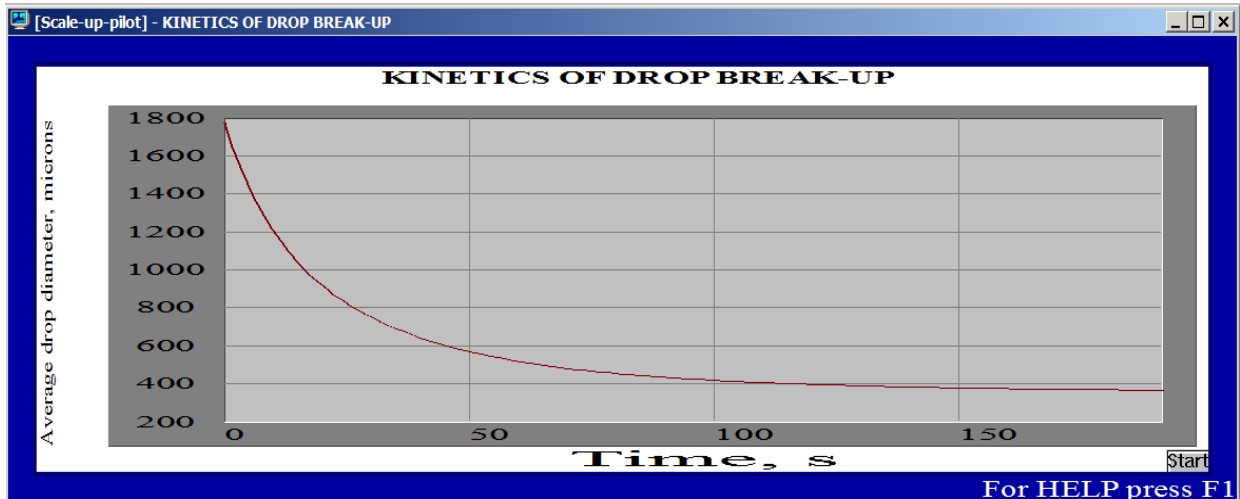
Figure 3-14. Kinetics of drop break-up. Pilot reactor.

The next process parameter you are interested in is **Specific mass transfer area**. To obtain this parameter, just click on **Last menu** in the main menu and select **Specific mass transfer area**. The result of the calculation is shown in Figure 3-15.

Figure 3-15. Specific mass transfer area. Pilot reactor.

Sometimes distribution of drops by diameter is important. Click on **Last menu** again, and select **Distribution of drops by diameter**. The result is shown in Figure 3-16.
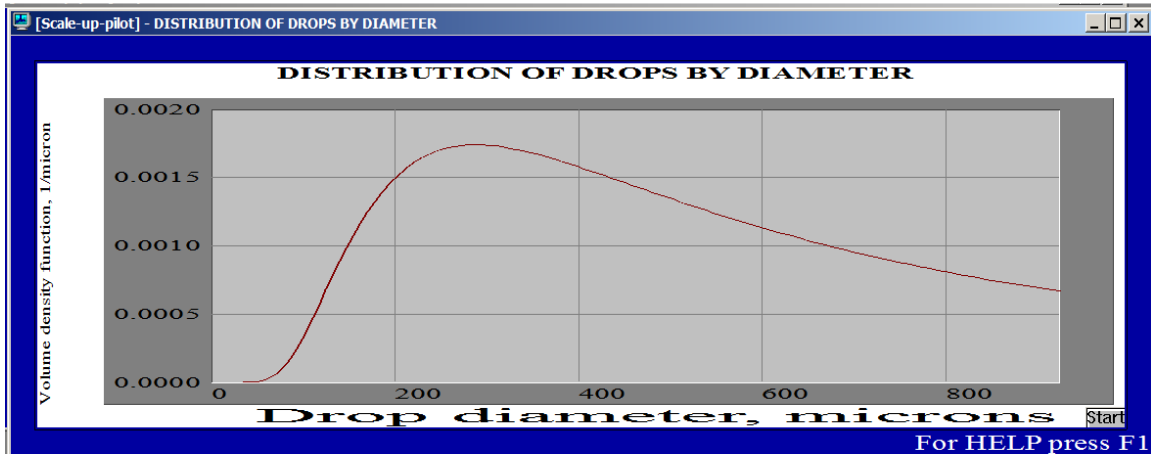
Figure 3-16. Distribution of drops by diameter. Pilot reactor.

The data in Figs 3-14 – 3-16 represents basic characteristics for a pilot reactor.

We recommend closing all windows before proceeding to calculations of production-scale reactor (**Window, Close All**).

Now let us enter the initial data for the available production-scale reactor. To do it, you may use the existing project and, using **Edit input** option in the main menu, change only those input tables that contain equipment characteristics. First save your current project, **Scale-up-pilot.vsm** then click on **Save as** option in the **Project** menu, and save your current project under a new name, for example, **Scale-up-production.vsm**

Now enter the data of your production-scale reactor. Let's start with the tank data. Click on **Edit input** - **Tank** - **Tank geometry** and supply the internal dimensions of the production-scale tank (Figure 3-17).

Select **Edit input** - **Baffles,** and then **Choose new baffle** at the bottom of the table that appears. In accordance with your initial data for the production-scale reactor, select **Tubular baffle-2** in the **Baffle types** screen (Figure 3-18).
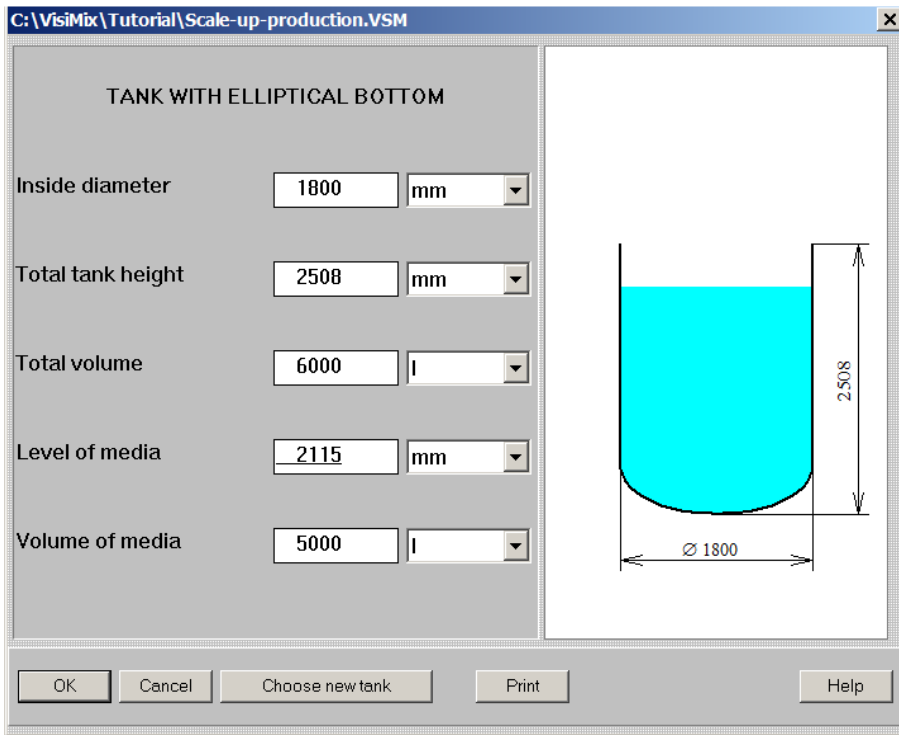
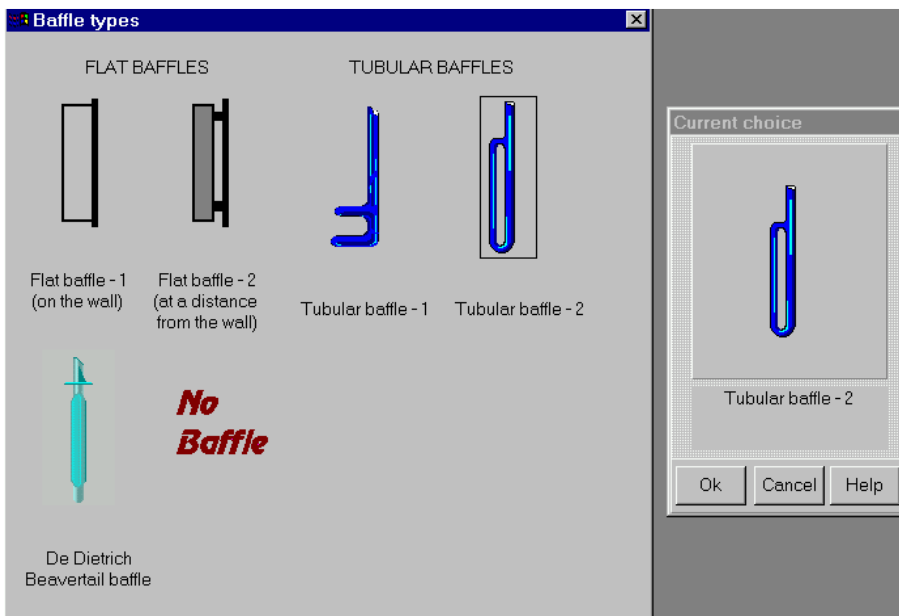**Figure 3-17. Entering data for production-scale tank.**

Figure 3-18. Selecting a baffle for the production-scale reactor.

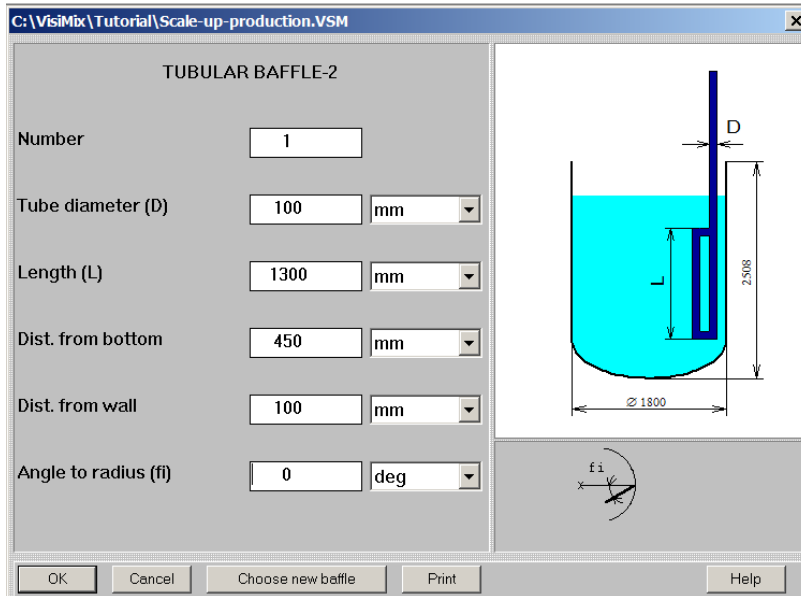Now enter the baffle characteristics based on the initial data given above (Figure 3-19).

Figure 3-19. Entering baffle data for the production-scale reactor.

Select **Edit input** - **Impeller**, and click on **Choose new impeller** at the bottom of the DISK TURBINE input table. In your production-scale reactor, you have a single-stage three-blade glass lined impeller. Select **GLASS LINED impeller–1** in the **Impeller types** screen (Figure 3-20), and **single** in the **Current choice** window on the right.

Enter the data for **GLASS LINED IMPELLER-1** agitator in the input table that appears (Figure 3-21).

Whenever you change the equipment parameters, the tank diagram changes reflecting your input. The diagram of your industrial tank corresponding to the data you have entered is shown in Figure 3-22.
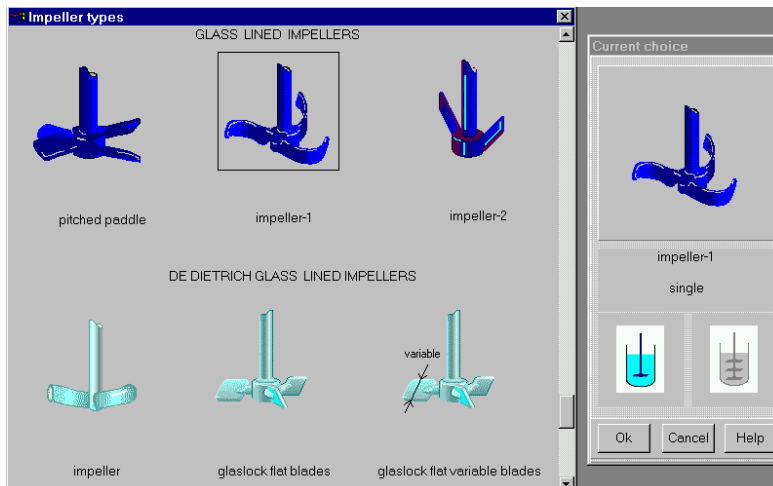

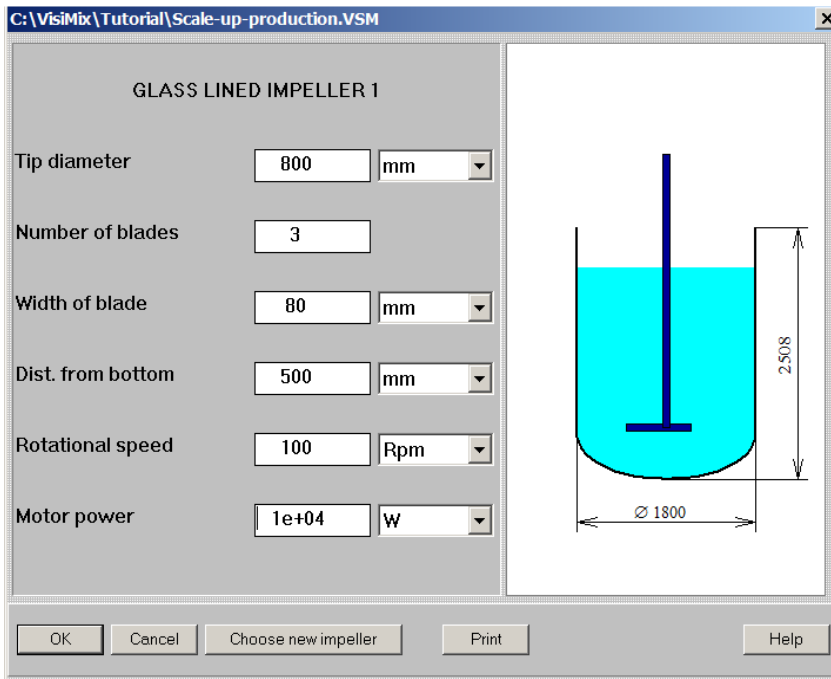*Figure 3-20. Selecting impeller for production-scale reactor.*

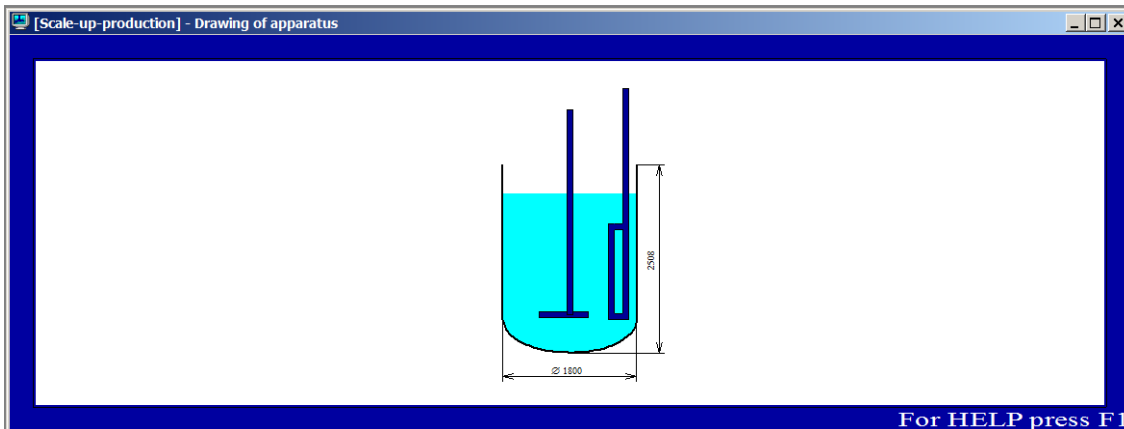**Figure 3-21. Entering impeller data for the production-scale reactor.**

Figure 3-22. Tank diagram for production-scale reactor.

Now you can return to calculations. Select **Last menu** in the main menu and click on **KINETICS OF DROP BREAK-UP.** The program analyzes the process in your production-scale reactor, finds the process conditions unsatisfactory and issues a message, recommending to increase the number of baffles (Figure 3-23). Then the message shown above in Figure 3-12 will appear, suggesting that you change your input first and then repeat the question.
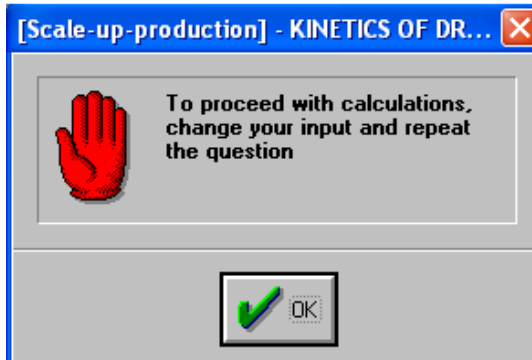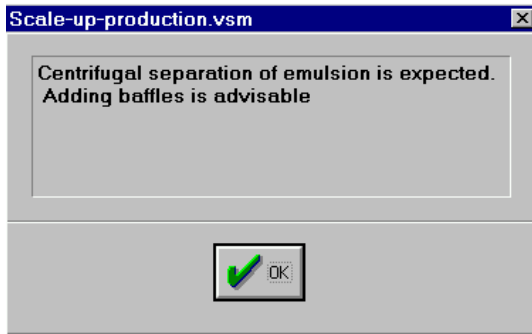
Figure 3-23. These messages recommend increasing the number of baffles in the available production-scale reactor.

To increase the number of baffles, select **Edit input** – **Baffles,** and change the number of baffles from 1 to 2 in the **Tubular baffle - 2** input table as shown in Figure 3-24.
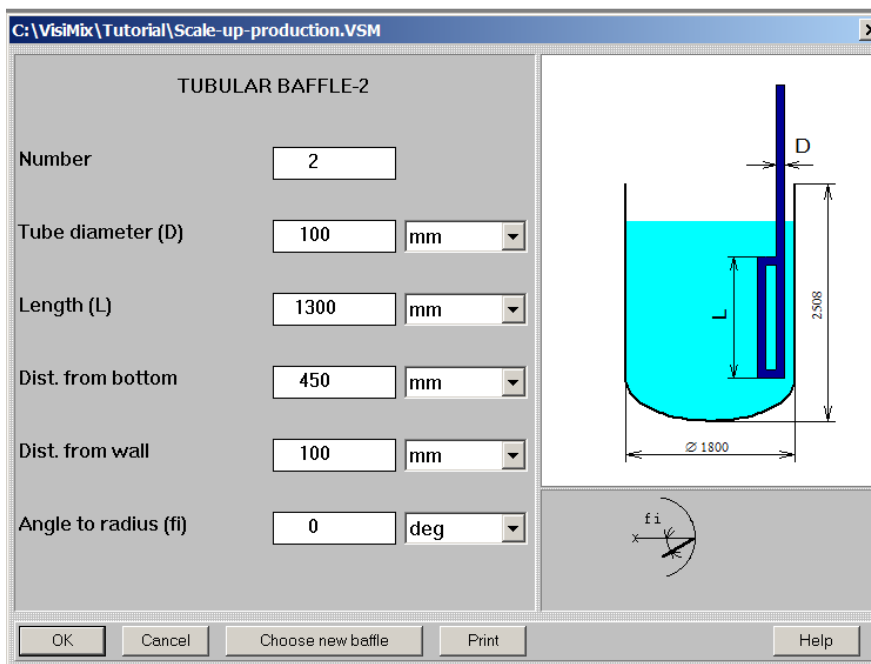

Figure 3-24. Adjusting baffle data for the production-scale reactor.

Select again **Last menu** in the main menu and click on **KINETICS OF DROP BREAK-UP.** You will not receive any warning message, which means that the operating

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conditions are now satisfactory. In a very short time, the calculations will be finished, and a graph of **Kinetics of drop break-up** will appear (Figure 3-25). From this graph, you can see that stabilization time for the industrial reactor is about 4-5 min.
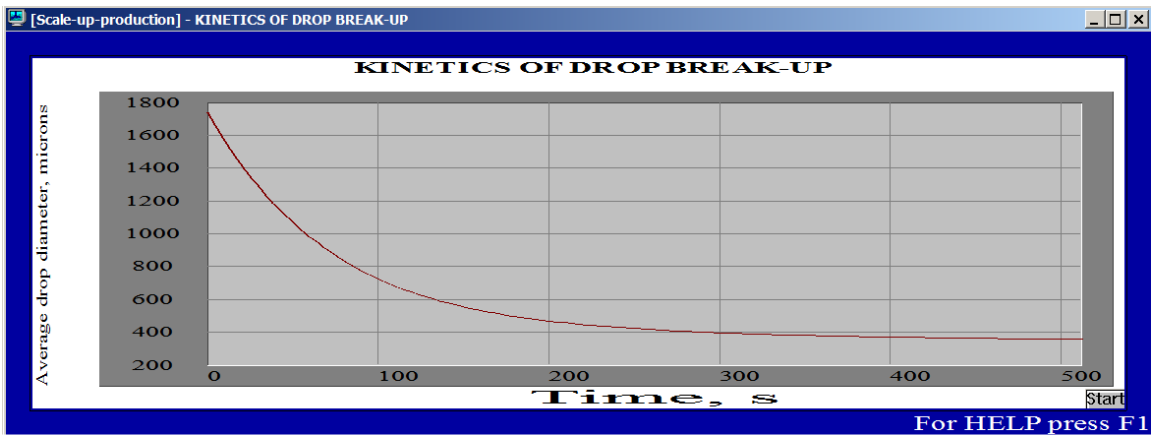

Figure 3-25. Kinetics of drop break-up. Production-scale reactor.

Now you must calculate the second process parameter required for scaling-up: **Specific mass transfer area**. Click on **Last menu** and select this parameter. The result is shown in Figure 3-26.

Use **Last menu** to obtain **Distribution of drops by diameter** (Figure 3-27).

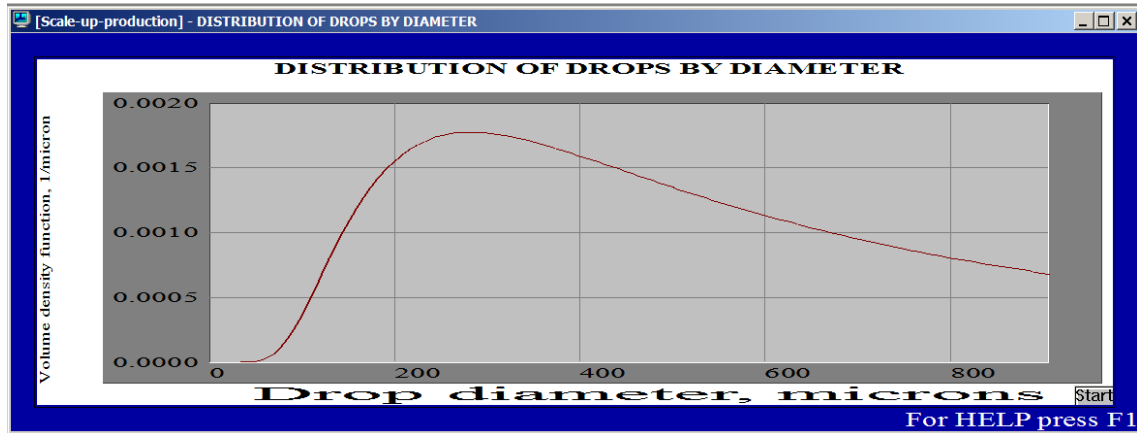*Figure 3-26. Specific mass transfer area. Production-scale reactor.*

Figure 3-27. Distribution of drops by diameter. Production-scale reactor.

The comparison of the pilot data (Figs 3-14 – 3-16) and the data for production-scale reactor (Figs 3-25 – 3-27) shows the following:

- The value for stabilization time is considerably less than 10 minutes for both reactors (2 minutes for pilot reactor and 5 minutes for production-scale reactor).

- Specific mass transfer area is practically the same for both reactors: 3450 m^2/m^3 for pilot reactor and 3520 m^2/m^3 for production-scale reactor).

- The distribution of drops by diameter is also practically identical for both reactors.

The conclusion:

Calculations for pilot and modified production-scale reactor show that emulsification processes in both reactors are similar, and the scaling-up can be successfully performed, provided that the available production-scale reactor is modified in accordance with the VisiMix recommendations.