VISIMIX TURBULENT. CRYSTALLIZER. SCALING-UP .

This example is based essentially on the article 'Optimizing Crystallizer Scaleup' by Wayne J. Genk , Chem. Engng. Progress, June 2003, pp. 36-44.

Problem description:

Accordingly to the existing views, the process rate and particle size distribution in crystallization and precipitation processes are dependent on chemical composition and physico-chemical properties of the system. In the same time thay can be
substantially dependent also on some phenomena that are functions of mixing conditions – for example, on primary and secondary nucleation, attrition and breakage of crystals, distribution of solid phase and liquid-solid mass transfer.
The following example is related to a particular case when the crystallization is controlled mainly by these parameters, and scaling-up conditions include reproduction of these phenomena.
The corresponding parameters selected from the list of VisiMix outputs and used below for crystallization scale-up are presented in the Table 1.

Table 1. Scaling-up parameters for crystallization.

VisiMix Menu section	Output parameters
	Energy dissipation – maximum value
	Turbulent shear rate near the impeller blade
	Relative residence time in zone with maximum dissipation
Liquid-solid mixing	**Axial and radial distributions of the solid phase**
	Maximum energy of collisions
	Frequency of collisions of maximum energy
Liquid –solid mass transfer	**Mass transfer coefficient**

Subject of this example – to illustrate application of VisiMix for scaling-up of the crystallization process based on these parameters.

For calculation of the **Mass transfer coefficient**, it is necessary to enter a number of additional initial data, including the **Diffusivity of the solute**. In our case the problem consists not in prediction, but in reproduction of the same value of the **Mass transfer coefficient**. For a given set of physical properties of the solution and solute, mass transfer coefficient is tightly connected to the **Average value of turbulent energy dissipation**. So, in this example we will use this parameter as a base for scaling-up instead of the **Mass transfer coefficient**.

Initial data

Pilot crystallizer:

Tank (with elliptical bottom):
Inside diameter = 650 mm;
Total volume = 231 liter (61 gal);
Volume of media = 190 liters (50 gal).

Baffle (Flat baffle-1)
Number = 4;
Width = 60 mm;
Length = 500 mm;
Distance from bottom = 150 mm;
Angle to radius = 0 deg.

Impeller (pitch paddle)
Tip diameter = 210 mm;
Number of blades = 3;
Pitch angle = 45 deg;
Width of blade = 40mm;
Distance from bottom = 125 mm;
RPM = 310;
Power of drive = 1000 W;

Production plant crystallizer

Tank (with elliptical bottom):
Inside diameter = 3000 mm;
Total volume = 26.5 m^3 (7000 gal);
Volume of media = 23.7 m^3 (6250 gal).

Baffles (Flat baffle-2)
Number = 4;
Width = 300 mm;
Length = 3200 mm;
Distance from bottom = 600 mm;
Distance from wall = 50 mm;
Angle to radius = 0 degrees

Impeller (A310)
Tip diameter = 1400 mm;
Distance from bottom = 700 mm;
RPM = 105;
Power of drive = 20 kW;

Media properties

The media is a suspension of crystals in a water mother solution.
Liquid phase properties:
Density = 1050 kg/cub. m;

Dynamic viscosity = 0.001 Pa*s;

Solid phase properties:

Mass concentration = 150 kg/cub.m;;
Density = 2300 kg/cub. m;
Average particle size = 150 micron;
Size of largest particles = 250 micron;

The Solution:

Before proceeding to calculations, let us create the projects corresponding to the pilot and production-scale reactor and enter design data for each of them. Start with the pilot simulation, and then consider the available production-scale reactor, changing its design characteristics if necessary.

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

Select **Project,** then **New,** then enter the name for project **Cryst-pilot.vsm** as shown in Figure 1.

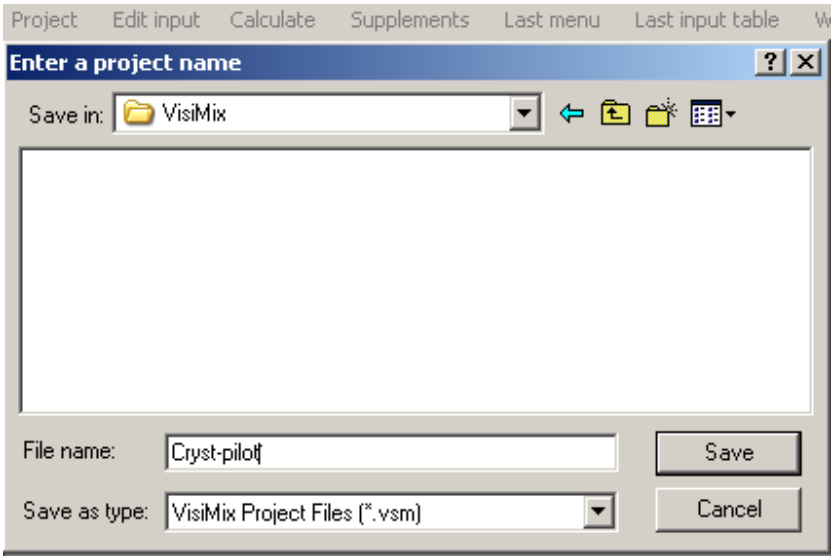


Figure 1. Starting a new project.

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 2). Click **OK** to confirm your choice.

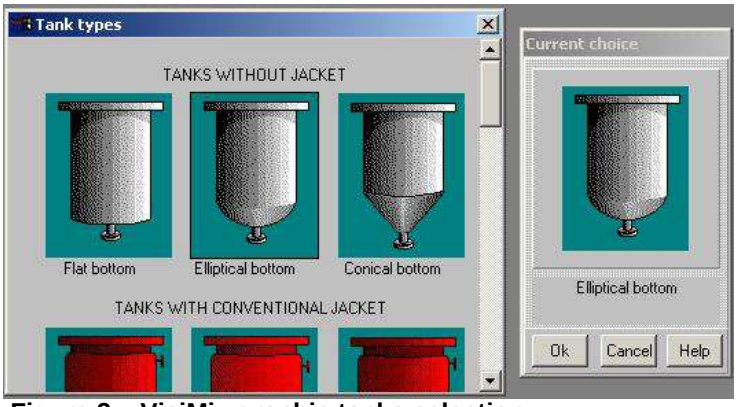


Figure 2. VisiMix graphic tanks selection.

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).

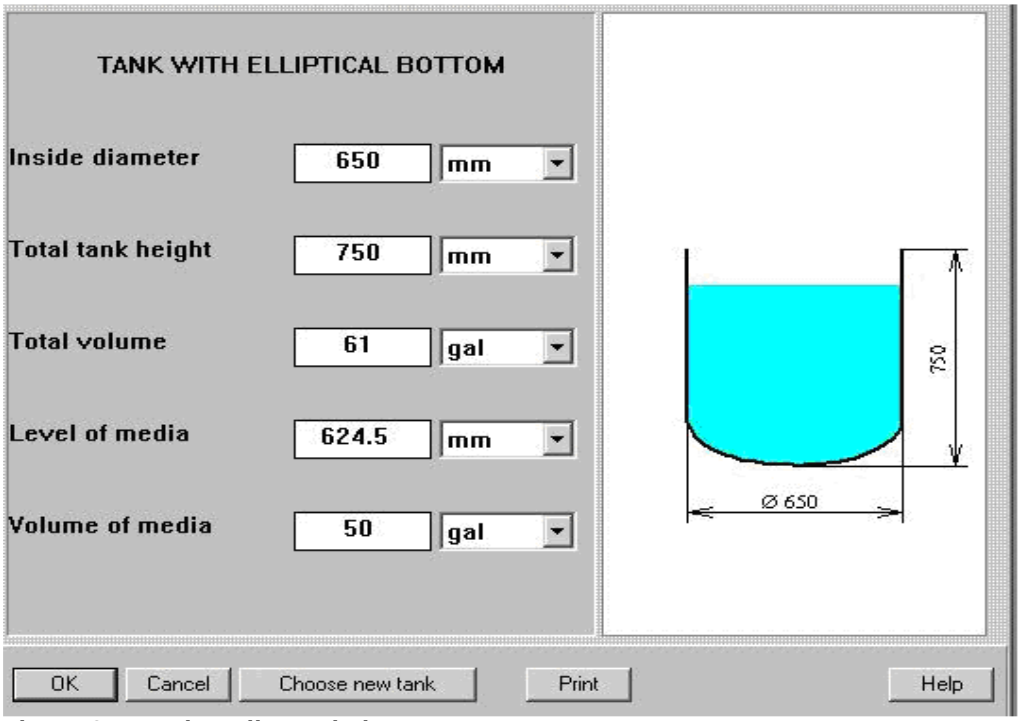


Figure 3. Entering pilot tank data.

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 – 1** in our case), and it will appear in the **Current choice** window on the right (Figure 4). Click **OK** to confirm the choice.

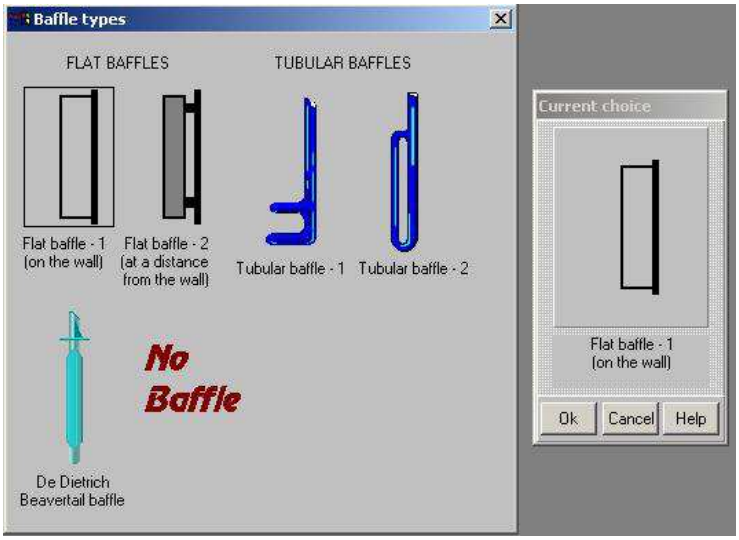


Figure 4. Selecting a baffle for pilot tank.

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

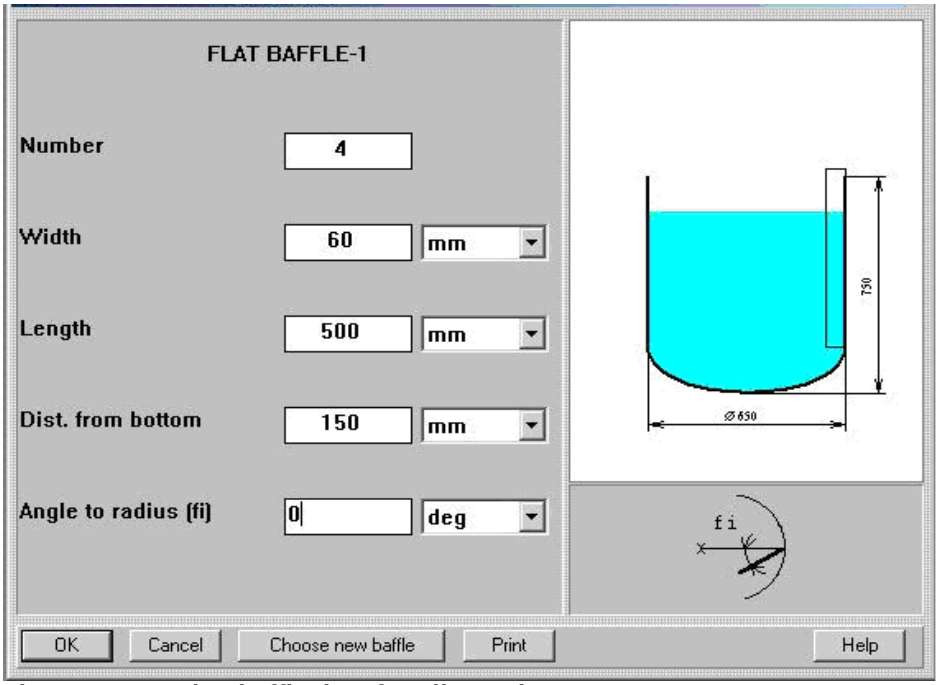


Figure 5. Entering baffle data for pilot tank.

Now click on the existing impeller of the pilot tank (**Pitched paddle**) in the **Impeller types** menu (Figure 6), and it will arrive in the **Current choice** window. The **single impeller** option (for single-stage mixing device) is already shown (by default).

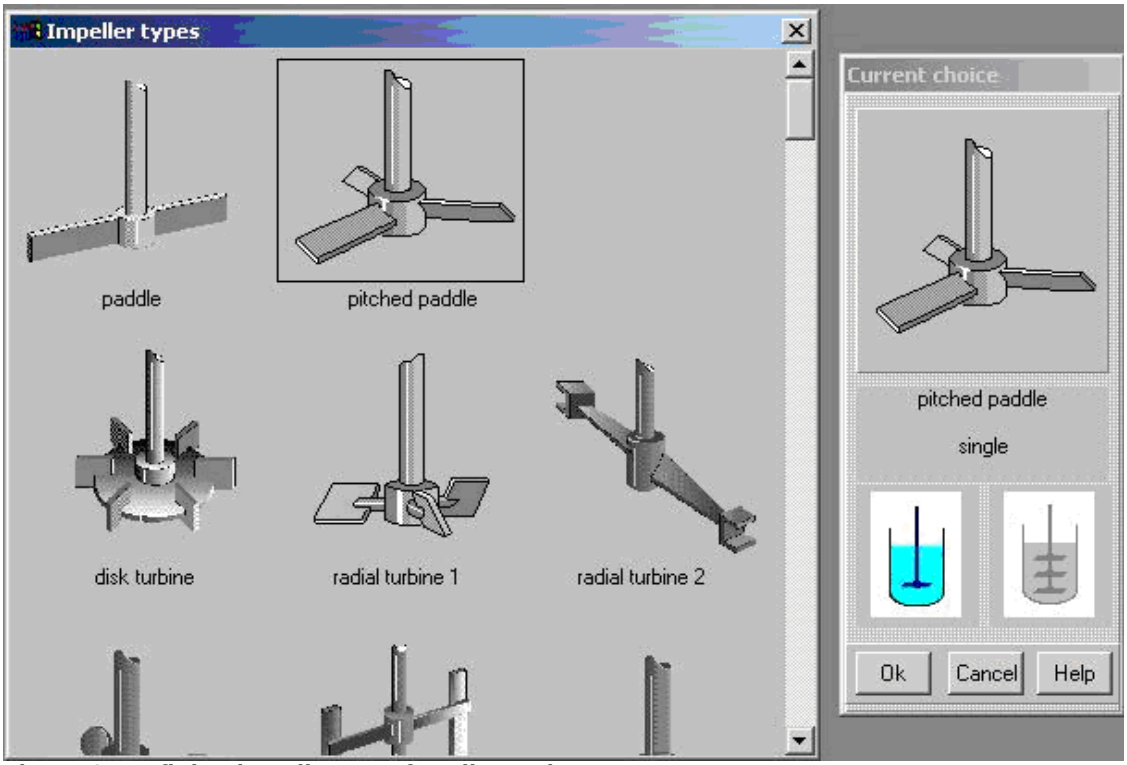


Figure 6. Defining impeller type for pilot tank.

The impeller parameters – sizes, position and rotation speed – are entered in the next input table that appears automatically (Figure 7). After the data are entered, click anywhere in the field of the window, and the diagram on the screen will change to reflect the last input. Click **OK** to confirm the input.

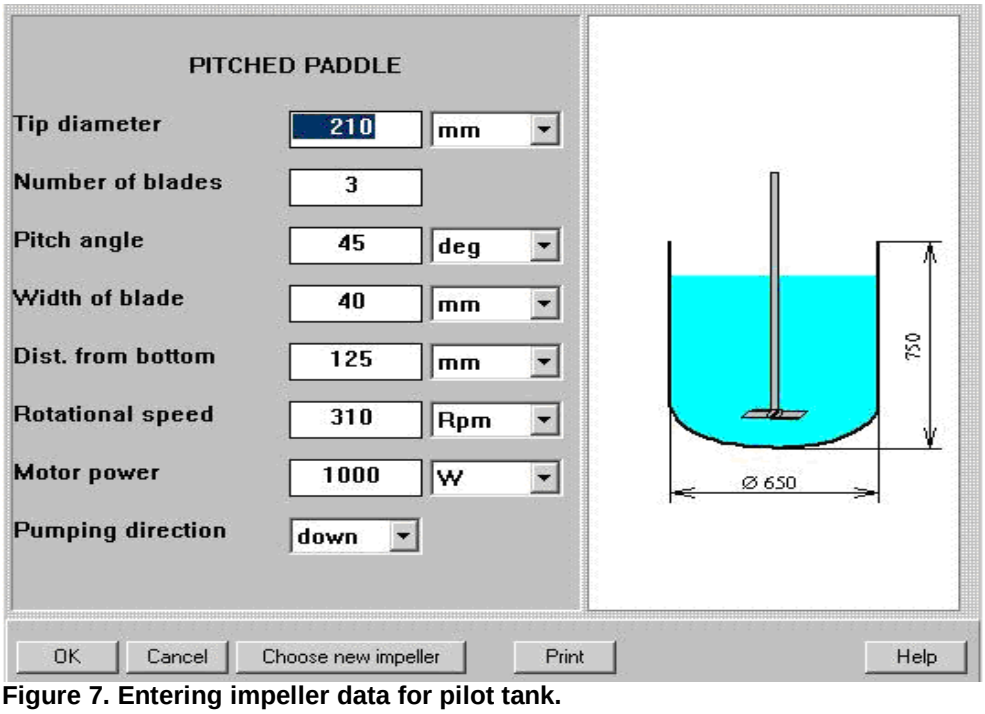


Figure 7. Entering impeller data for pilot tank.

You will now be requested to enter properties of the media in AVERAGE PROPERTIES OF MEDIA input table. For the first approximation, enter properties of the liquid phase ('mother solution').

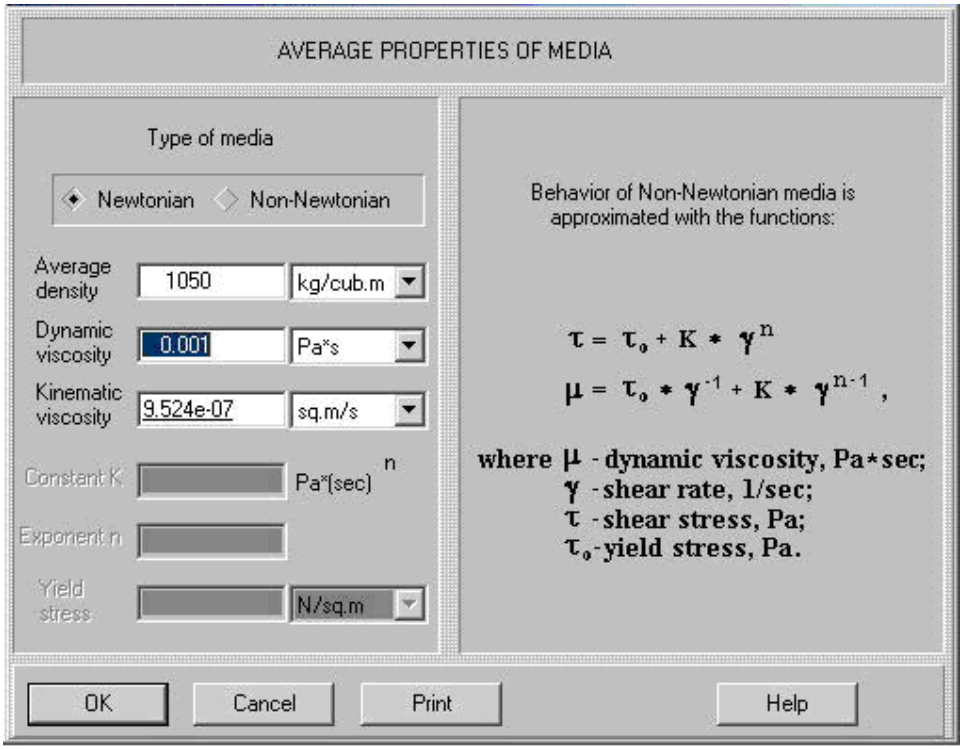


Figure 8. Entering average properties of media.

After you have entered basic data for your pilot reactor, its diagram appears (Figure 8).

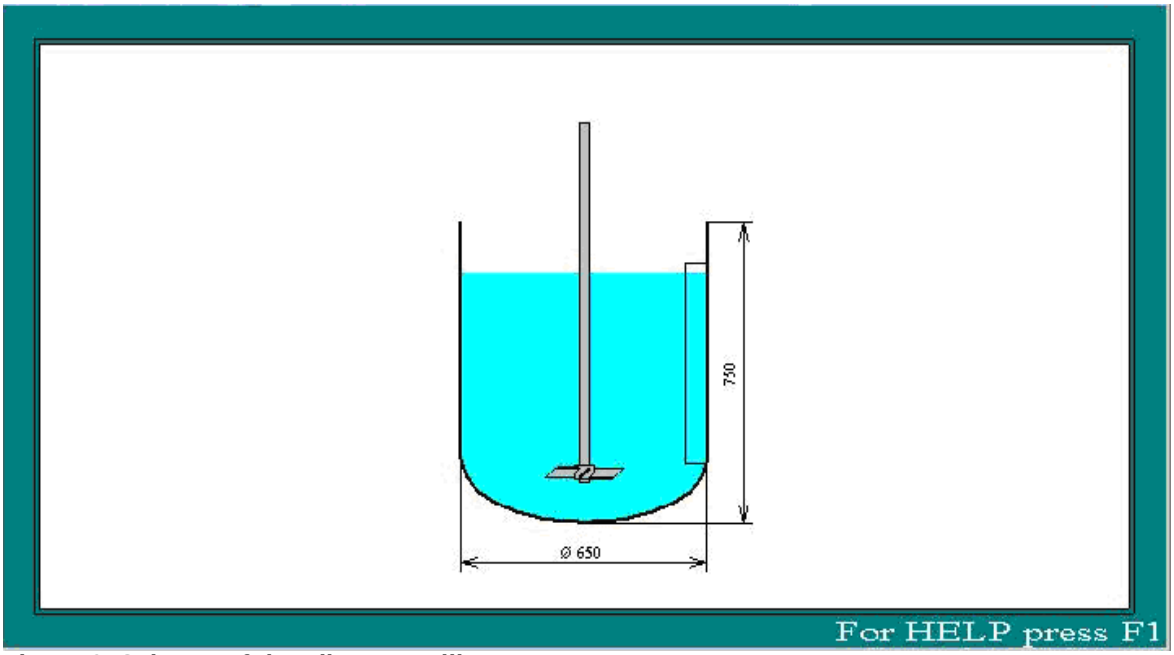


Figure 9. Scheme of the pilot crystallizer..

From now on, it is possible to start calculations.

The first stage of calculation – defining values of the controlling parameters for the pilot tank. In accordance with the Table 1, we will start with parameters of turbulence.

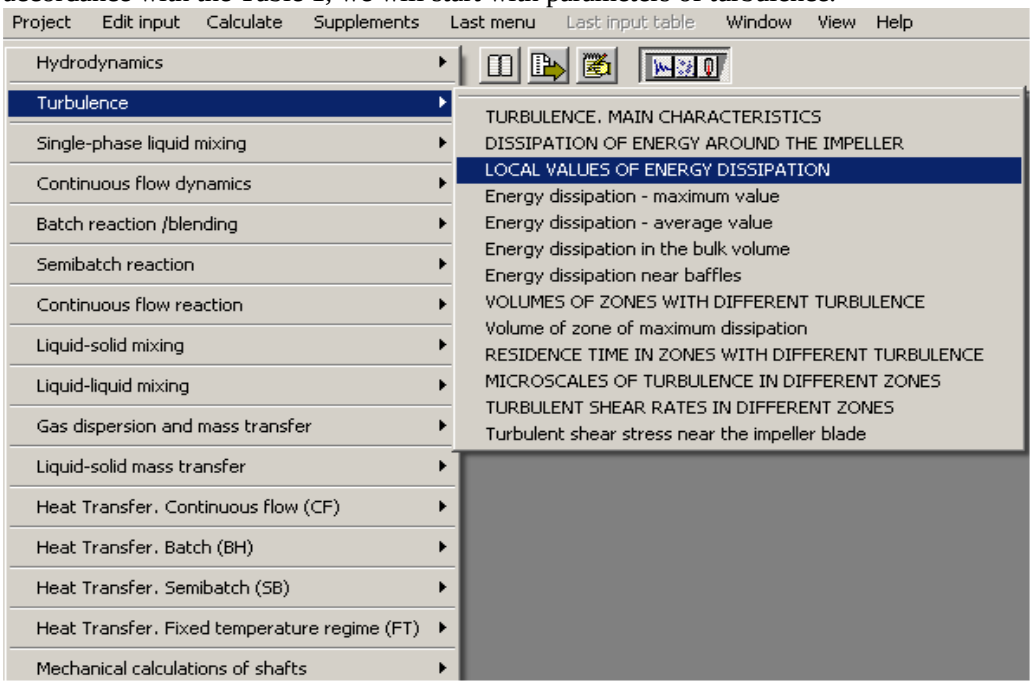


Figure 10. Menu Turbulence - list of output parameters.

Click the **Calculate** option in the main menu, select the sub-menu **Turbulence** (Figure 10) and 'ask' for **LOCAL VALUES OF ENERGY DISSIPATION** in this submenu. Output table containing the parameters **Energy dissipation – maximum value** and **Energy dissipation – average value** will appear (Figure 11).

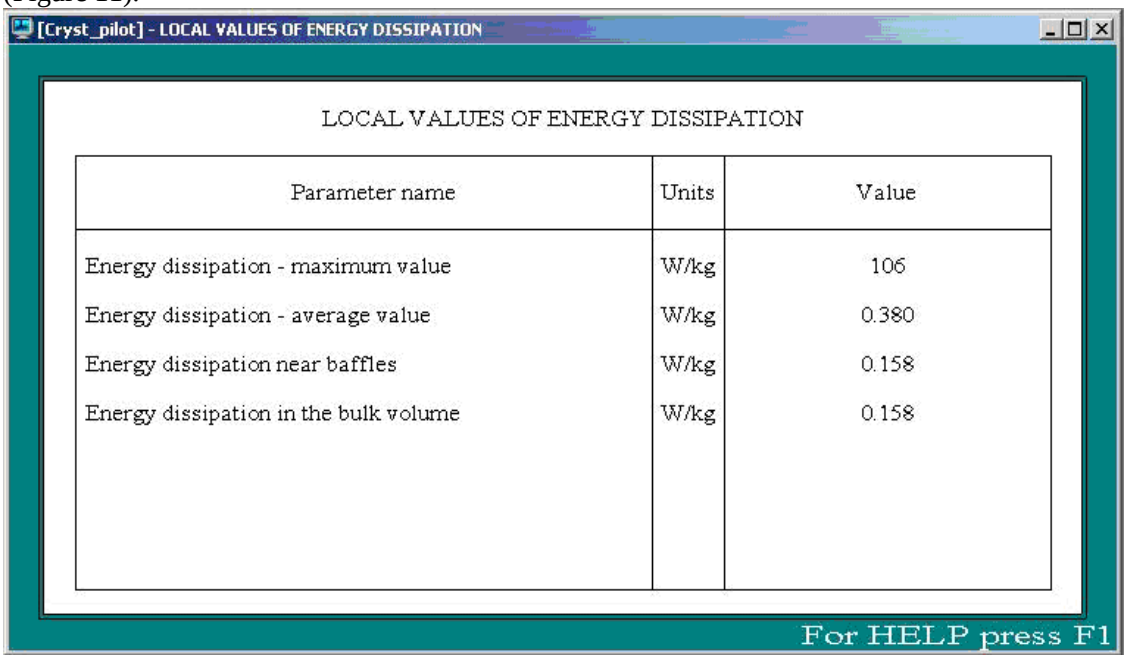


Figure 11. Pilot crystallizer. Local values of energy dissipation.

The next steps: select **Last menu** (Figure 12) and click the lines **TURBULENT SHEAR RATES IN DIFFERENT ZONES** and **RESIDENCE TIME IN ZONES WITH DIFFERENT TURBULENCE** in **TURBULENCE** section.

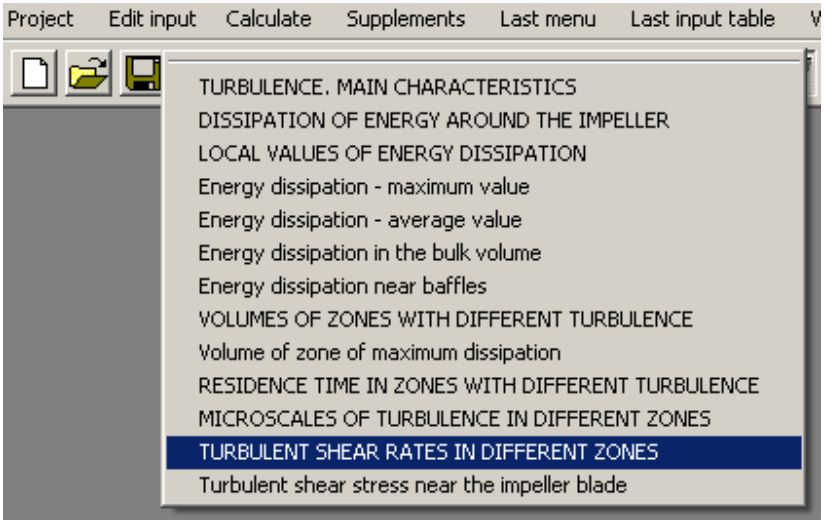


Figure 12. Menu Turbulence as the Last menu option.

The output tables (Figures 13 and 14) corresponding to these groups of parameters will appear on the screen.

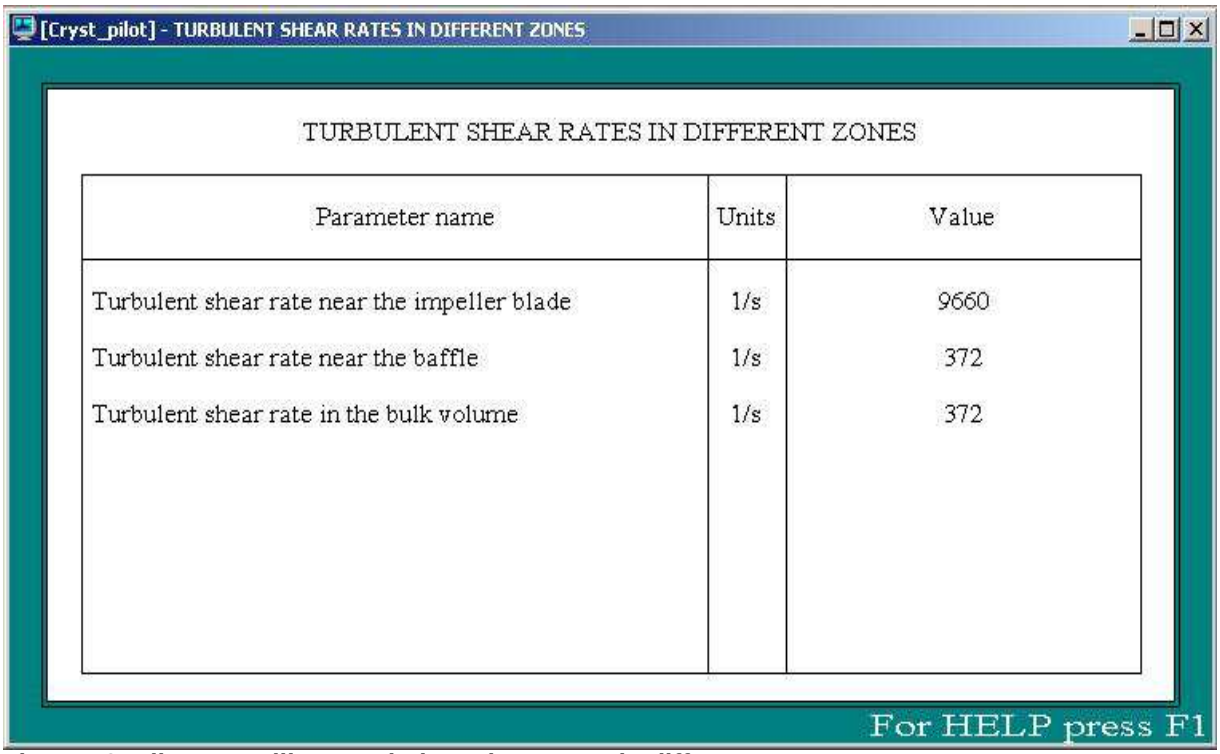


Figure 13. Pilot crystallizer. Turbulent shear rates in different zones.

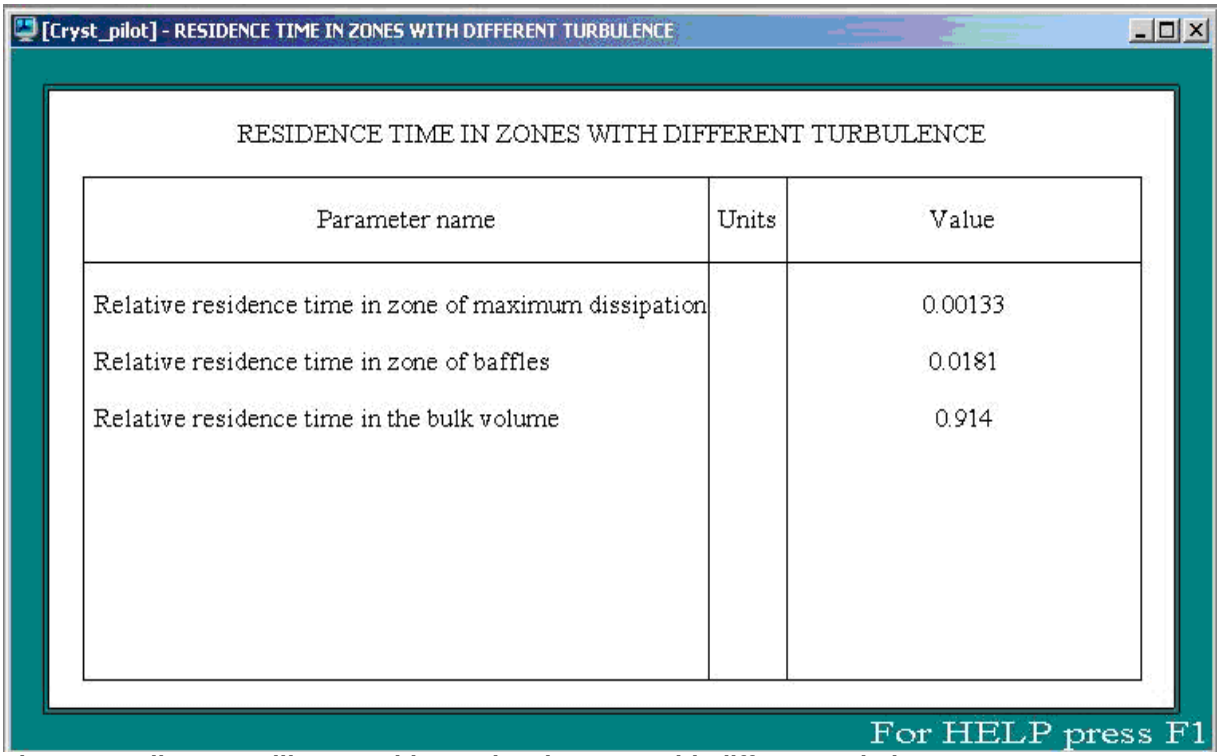


Figure 14. Pilot crystallizer. Residence time in zones with different turbulence

Accordingly to the Table 1, the next stage of our calculations is based on simulation of mixing in liquid-solid system.

To proceed, select **Calculate** in the main menu and click on **Liquid-solid mixing**. A sub-menu corresponding to this simulation step will appear (Figure 15). Select this option **LIQUID-SOLID MIXING. MAIN CHARACTERISTICS** in this sub-menu.

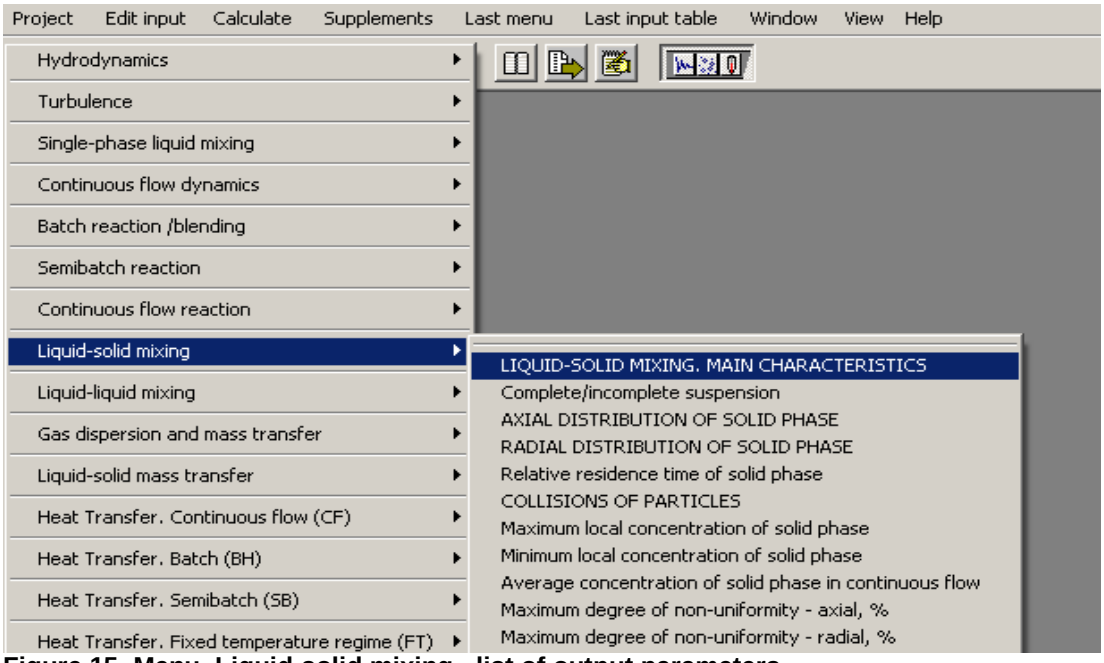


Figure 15. Menu Liquid-solid mixing - list of output parameters.

As a response, the program provides an input table for additional initial data (Figure 16).

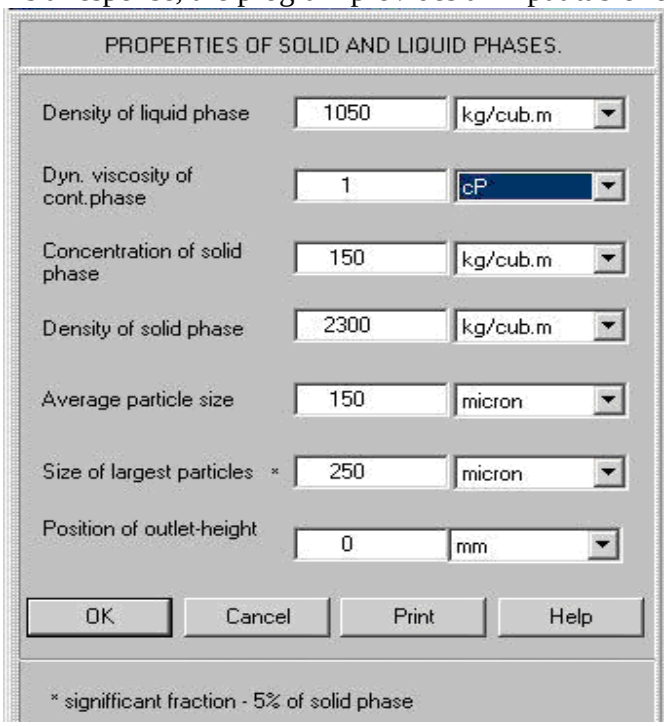


Figure 16. Entering of properties of solid and liquid phases.

Based on this information, VisiMix re-calculates the average properties of the media. If the calculated values do not correspond to the data entered earlier, you receive a message shown in Figure 17.

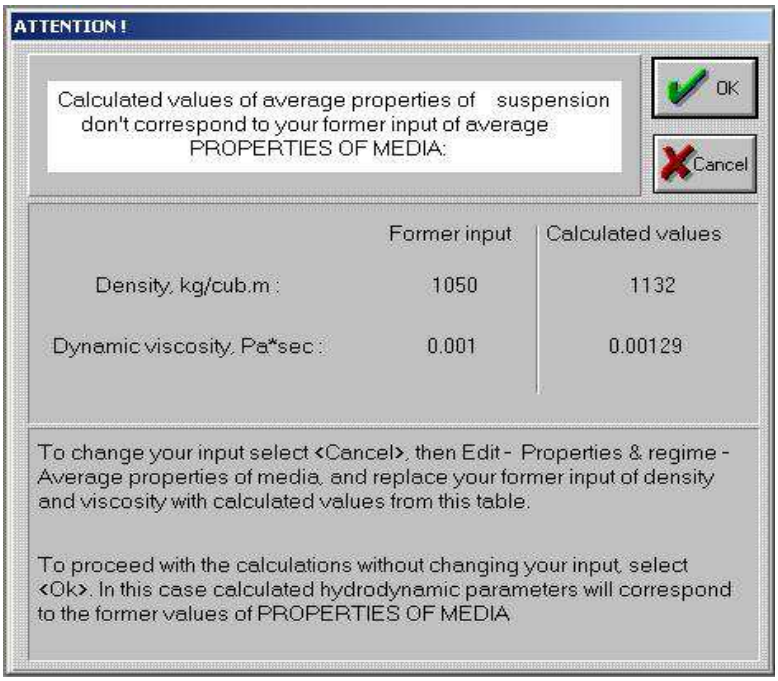


Figure 17. A warning of the discrepancy between entered and calculated average media properties.

Let's follow VisiMix recommendations and correct the data entered in the table **AVERAGE PROPERTIES OF MEDIA**. (Figure 18).

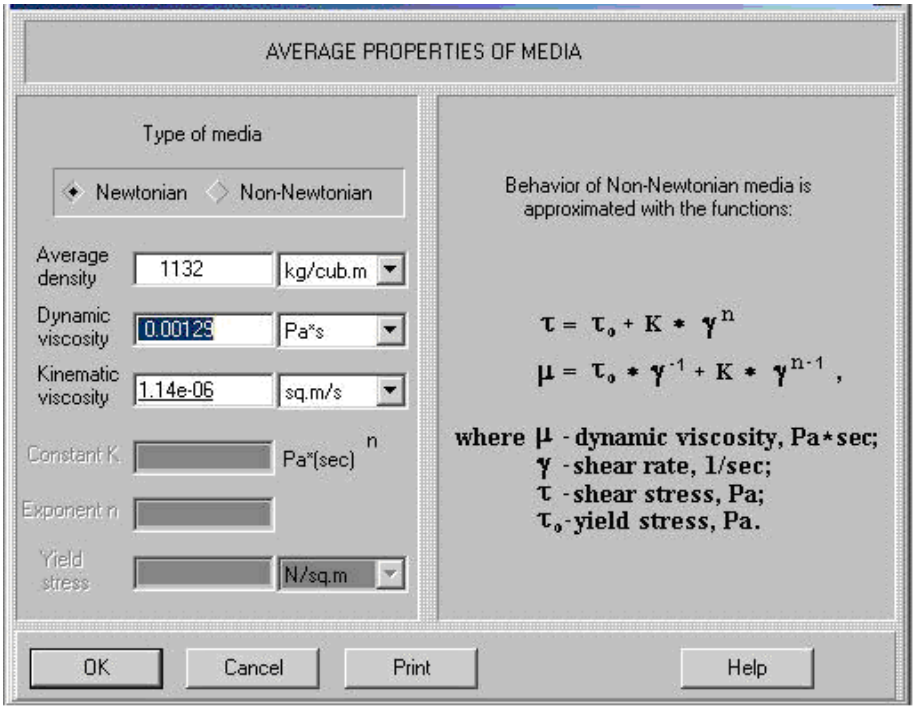


Figure 18. Adjusted average properties of media.

After the corrected figures have been entered, the program performs simulation and returns the calculated results table (Figure 19) corresponding to the requested output option.

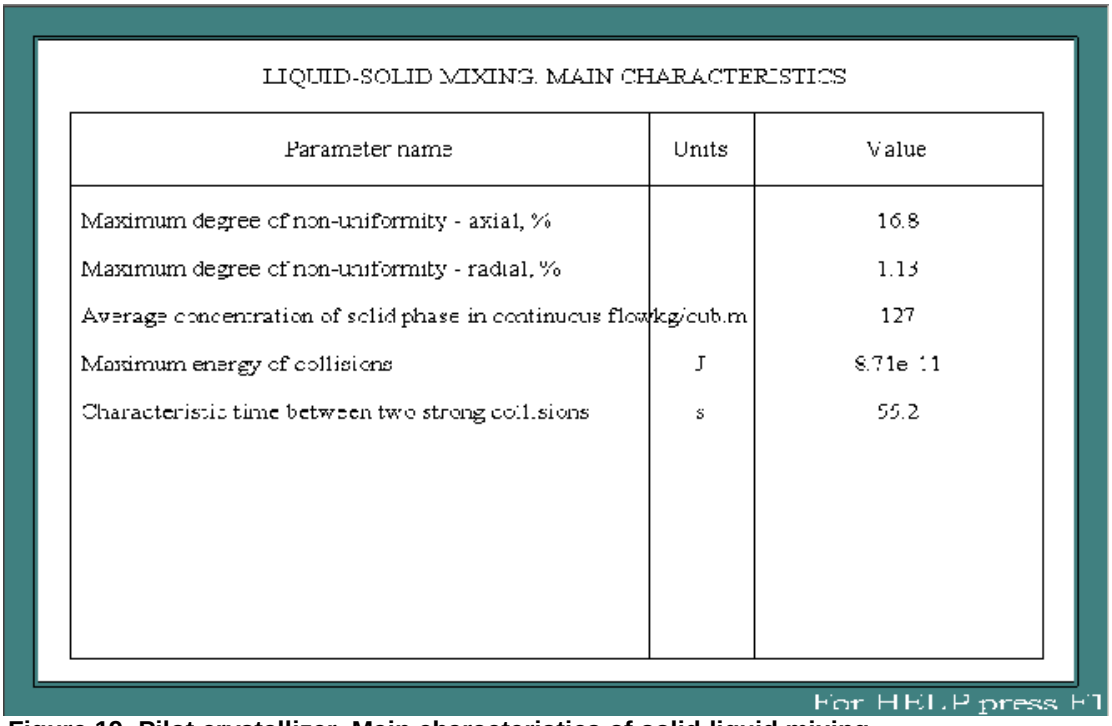


Figure 19. Pilot crystallizer. Main characteristics of solid-liquid mixing.

The next step – select **Last menu** and click **COLLISIONS OF PARTICLES** in the **Liquid-solid mixing** section. The corresponding table (Figure 20) will arrive.

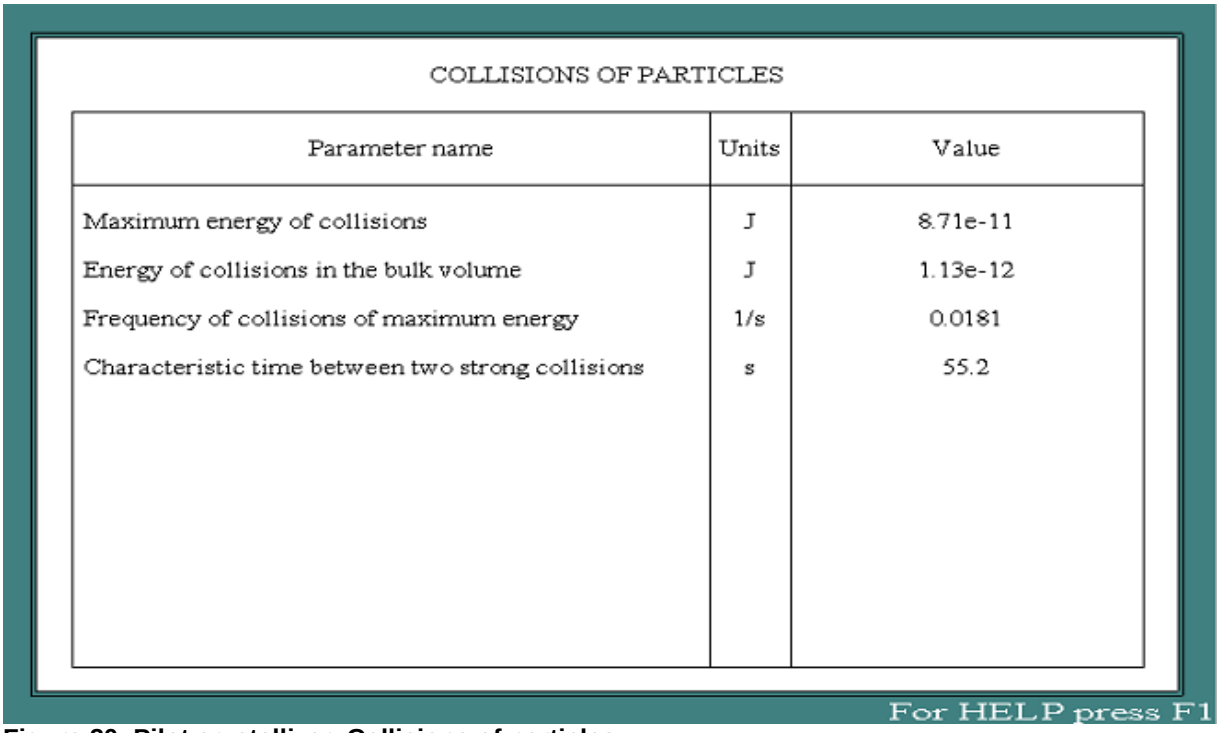


Figure 20. Pilot crystallizer. Collisions of particles.

The next stage of calculations – evaluation of mass transfer coefficient to suspended solid particles. Click **Calculate > Liquid-solid mass transfer** (Figure 21).

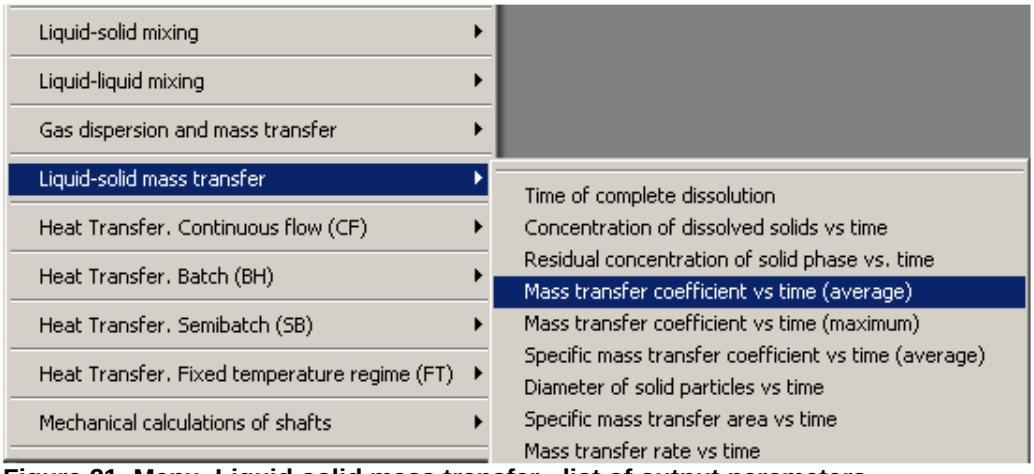


Figure 21. Menu Liquid-solid mass transfer - list of output parameters.

This sub-menu covers simulation of dissolution kinetics. Our goal is limited to comparison of mass transfer coefficients in two different crystallizers, so we select the output option **Mass transfer coefficient vs time (average).** Additional information on solubility of solid and concentration of the mother solution has to be entered. Taking into account the goal of our mass transfer calculations, we may enter some approximate values of these parameters, and also approximate value of diffusivity (Figure 22).

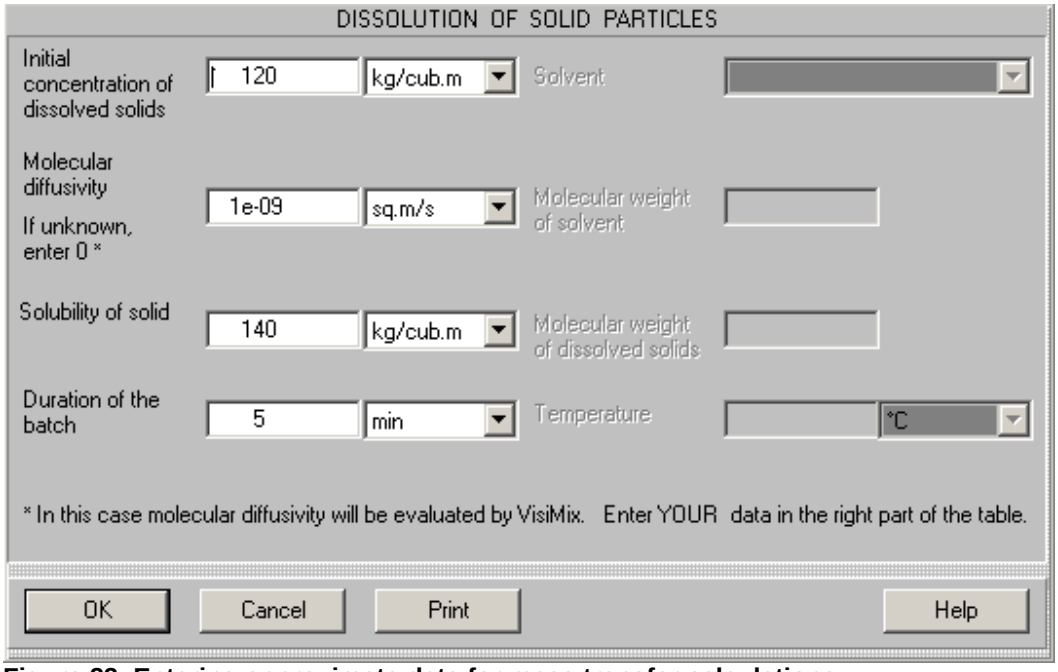


Figure 22. Entering approximate data for mass transfer calculations.

Result of calculation returned in a form of graph (Figure 23).The numerical value of the calculated parameter is presented in the VisiMix report for this project (see Help).

Figure 23. Pilot crystallizer. Mass transfer coefficient.

Based on the output data presented tables in Figures 11,13,14,19,20 and 23, we can prepare a table for comparison of the pilot and production scale crystallizers. On this stage only the column related to the pilot crystallizer is filled (Table 2).

Table 2. Comparizon of the pilot and production scale crystallizers.
Data for pilot crystallizer.

Menu section	Parameter	Pilot	Production
Turbulence	Energy dissipation – maximum value	106 W/kg	
	Turbulent shear rate near the impeller blade	9660 1/s	
	Relative residence time in zone with maximum dissipation	0.00133	
	Energy dissipation – average value	0.380 W/kg	
Liquid-solid mixing	Maximum degree of non-uniformity- axial	16.8%	
	Maximum degree of non-uniformity- radial	1.13%	
	Maximum energy of collisions	8.71e-11 J	
	Frequency of collisions of maximum energy	0.0181 1/s	
Liquid-solid mass transfer	Average mass transfer coefficient (approx.)	0.000038 m/s	

The data included in the Table 2 represent basic characteristics for the pilot crystallizer.

Now let us enter the initial data for the available production-scale mixing tank that is supposed to be used as a plant crystallizer. It is assumed that physical properties and regime parameters of the two crystallizers are identical, and only size and design is different. So, we can rename the existing project and change the equipment characteristics – Tank, Baffles and Impeller – accordingly to the technical characteristics of the production scale tank presented above (Figures 24-26).

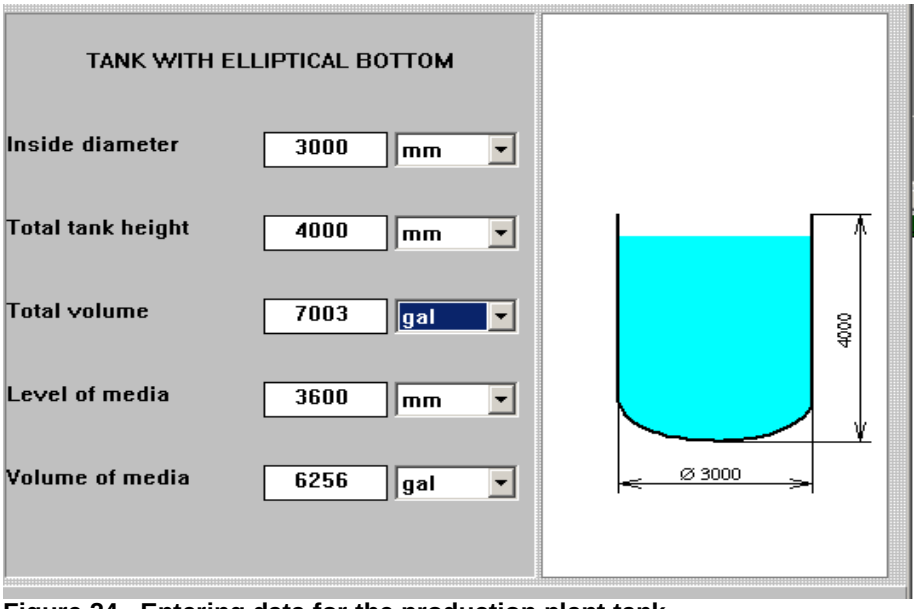


Figure 24. Entering data for the production plant tank.

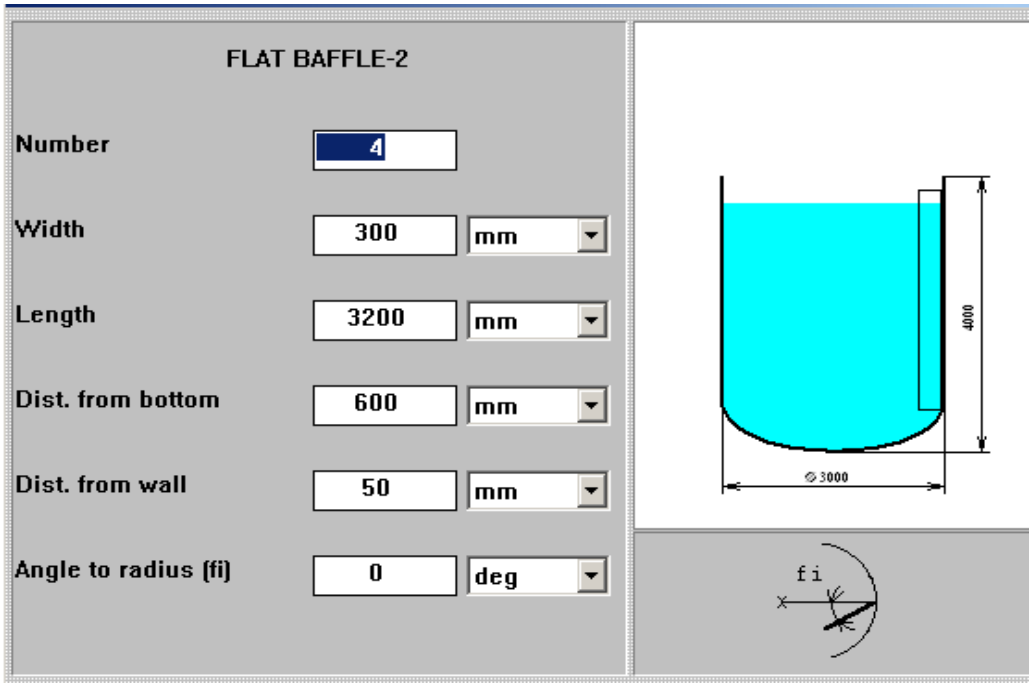


Figure 25. Entering baffles for the production plant tank.

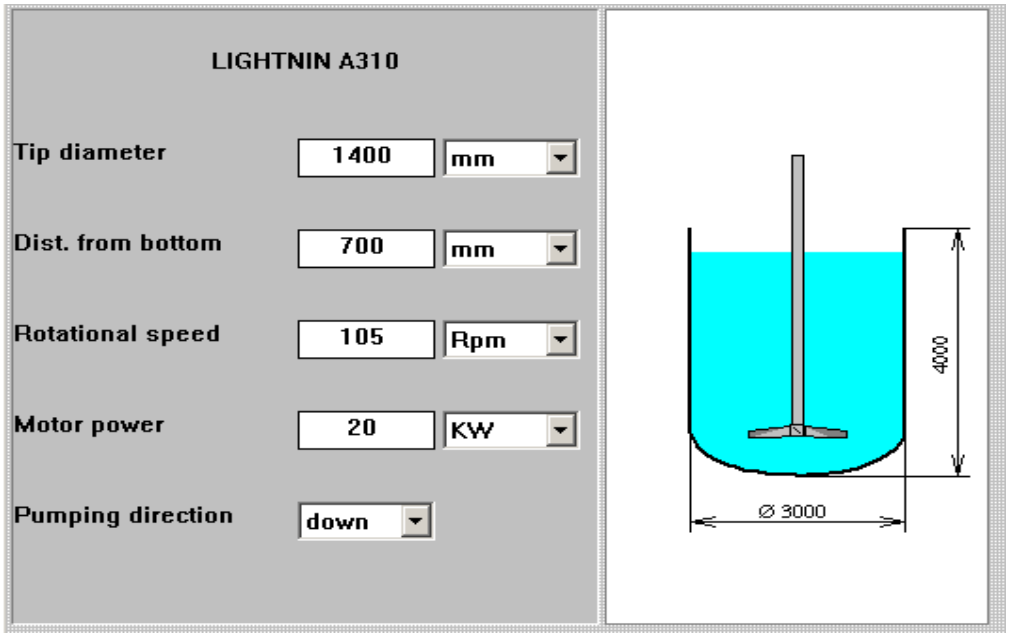


Figure 26. Entering agitator A310 for the production plant tank.

The diagram of the production plant tank is shown in Figure 27. Save the current project under a new name, for example, **Cryst-production.vsm.**

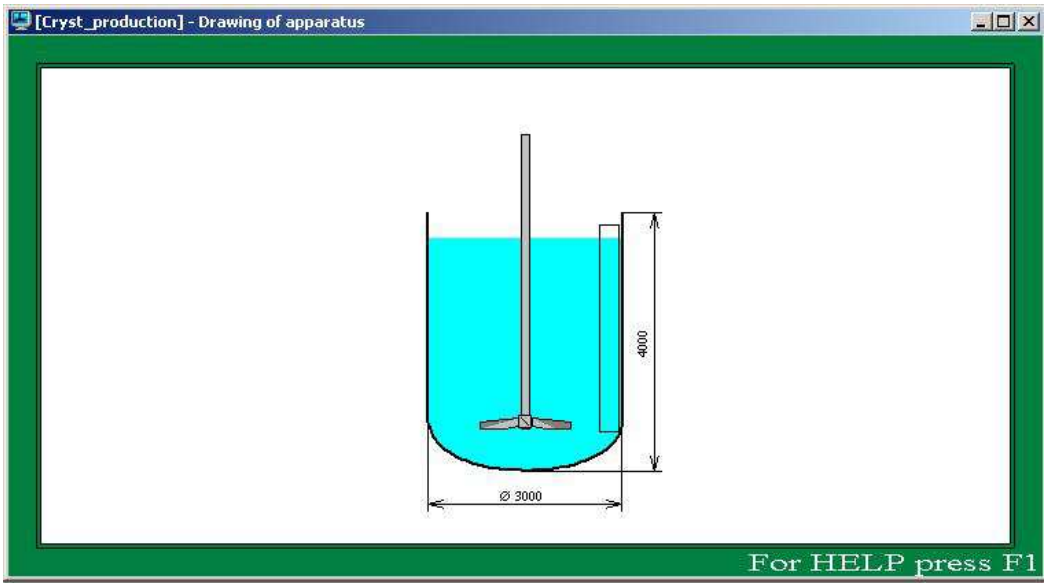


Figure 27. Diagram of the production plant tank.

Now we return to calculations. In order to compare the relevant parameters of the crystallizers, we perform calculations for the production tank in the same order as it has been done for the pilot tank.

Select **Turbulence** in the main menu and click **LOCAL VALUES OF ENERGY DISSIPATION.** A table containing the parameters **Energy dissipation – maximum value** and **Energy dissipation – average value** will appear (Figure 28).

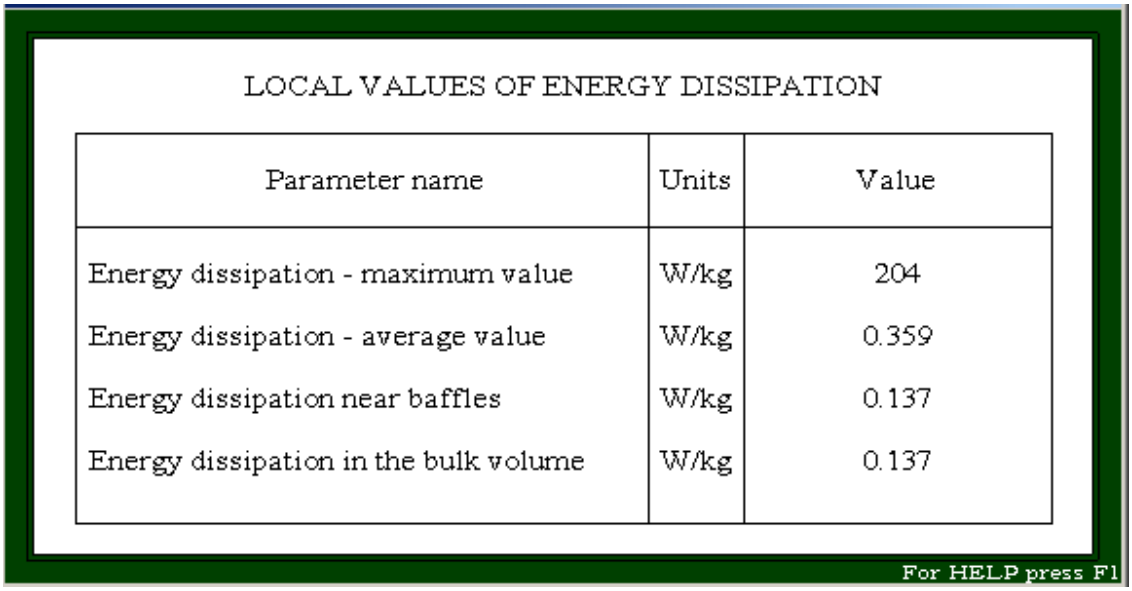
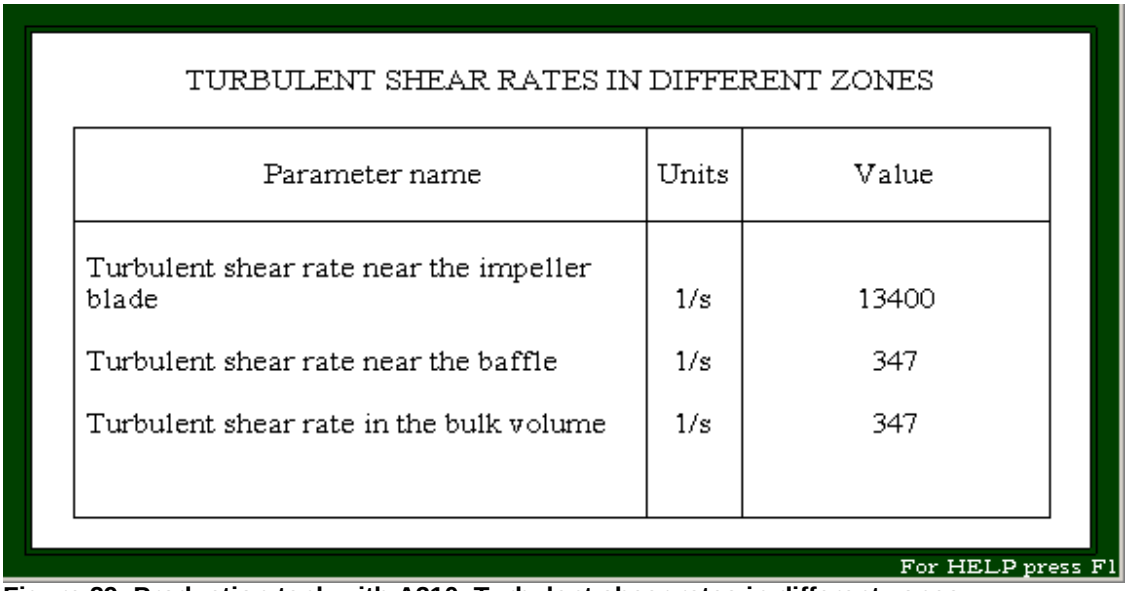


Figure 28. Production tank with A310. Local values of energy dissipation.

TURBULENT SHEAR RATES IN DIFFERENT ZONES and **RESIDENCE TIME IN ZONES WITH DIFFERENT TURBULENCE** in **Turbulence** section.

The tables (Figures 29 and 30) corresponding to these groups of parameters will appear on the screen.

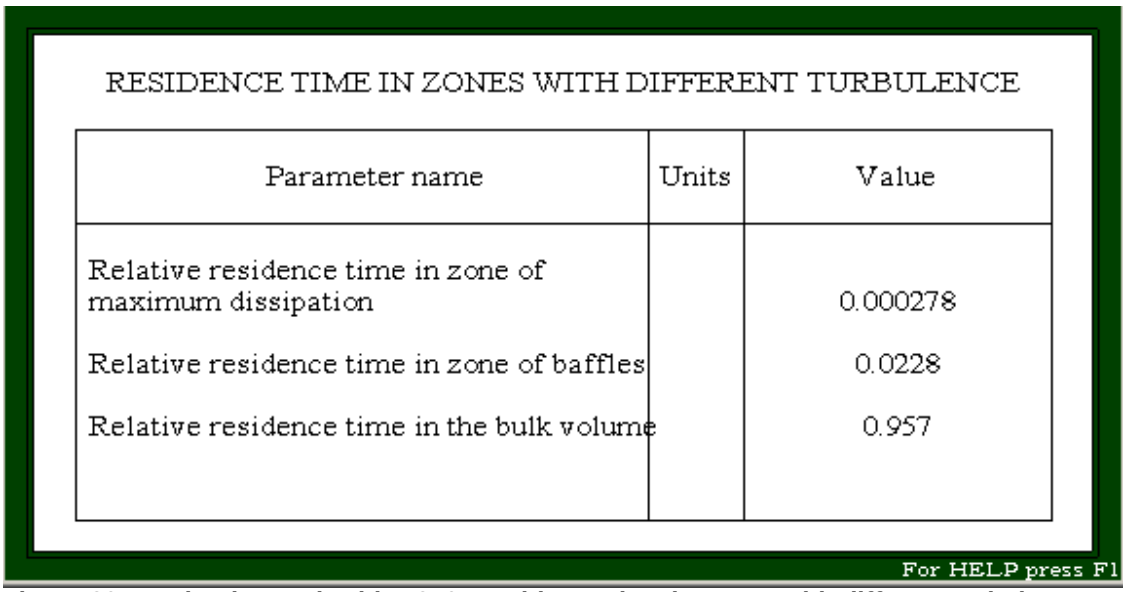


TURBULENT SHEAR RATES IN DIFFERENT ZONES

Parameter name	Units	Value
Turbulent shear rate near the impeller blade	1/s	13400
Turbulent shear rate near the baffle	1/s	347
Turbulent shear rate in the bulk volume	1/s	347

For HELP press F1

Figure 29. Production tank with A310. Turbulent shear rates in different zones.



RESIDENCE TIME IN ZONES WITH DIFFERENT TURBULENCE

Parameter name	Units	Value
Relative residence time in zone of maximum dissipation		0.000278
Relative residence time in zone of baffles		0.0228
Relative residence time in the bulk volume		0.957

For HELP press F1

Figure 30. Production tank with A310. Residence time in zones with different turbulence.

In the menu section **Liquid-Solid mixing** select **LIQUID-SOLID MIXING. MAIN CHARACTERISTICS** and get the calculated parameters (Figure 31) on the screen.

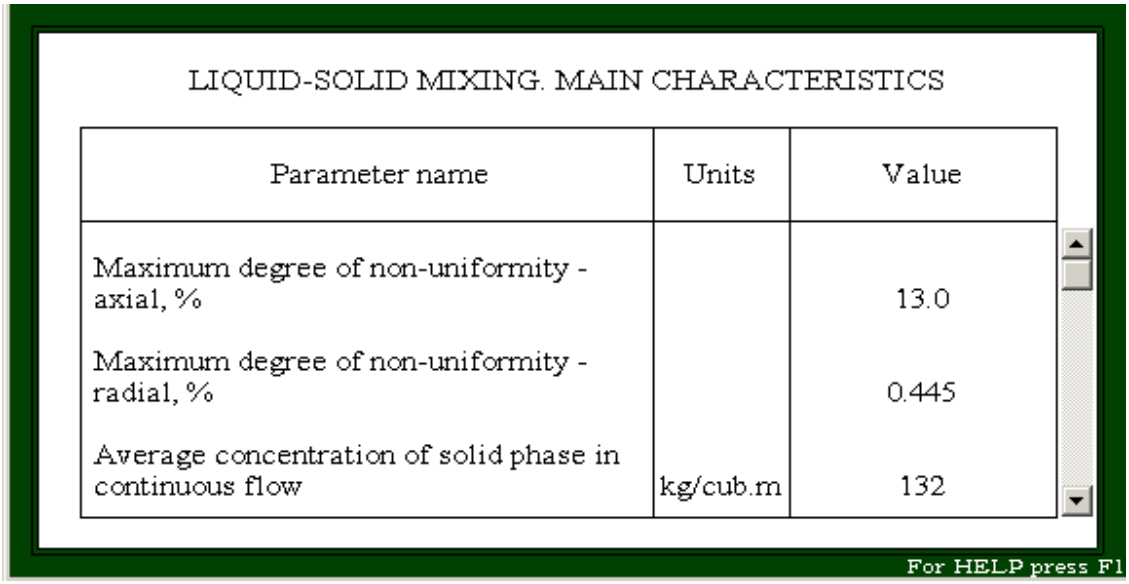


Figure 31. Production tank. Liquid-solid mixing. Main characteristics.

The next step – select **Last menu** and click **COLLISIONS OF PARTICLES** in the **Liquid-solid mixing** section. The corresponding table (Figure30) will arrive.

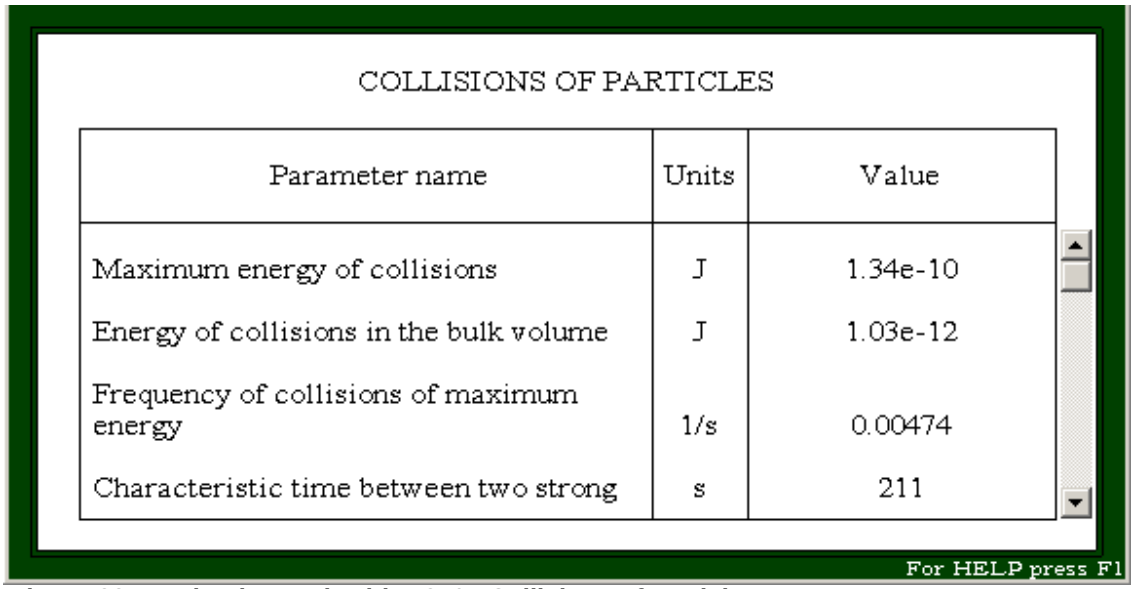


Figure 32. Production tank with A310. Collisions of particles.

The last step – calculation of mass transfer coefficient via Calculate>Liquid-solid mass transfer>Mass transfer coefficient vs time (average) (Figure 33).

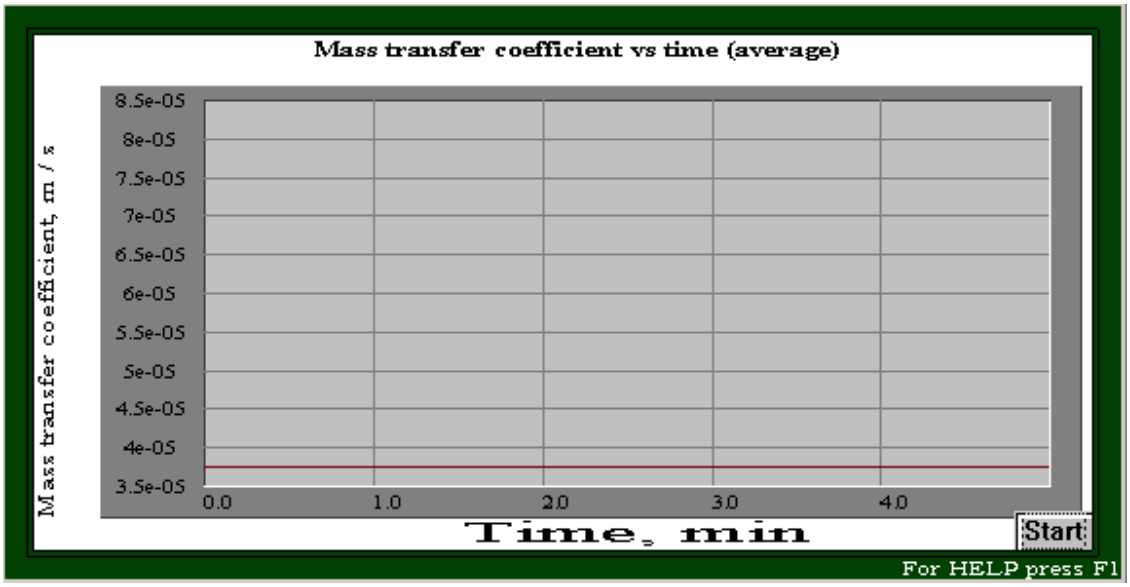


Figure 33. Production tank with A310. Mass transfer coefficient.

Based on the obtained results, we can print the calculated parameters for the plant tank into the Table 2 and compare them with the corresponding parameters of the pilot crystallizer (see Table 2a).

Table 2a. Comparison of the pilot crystallizer and production scale tank with A310.

Menu section	Parameter	Pilot	Production with A310
Turbulence	Energy dissipation – maximum value	106 W/kg	204
	Turbulent shear rate near the impeller blade	9660 1/s	13400
	Relative residence time in zone with maximum dissipation	0.00133	0.000278
	Energy dissipation – average value	0.380 W/kg	0.359
Liquid-solid mixing	Maximum degree of non-uniformity- axial	16.8%	13.0
	Maximum degree of non-uniformity- radial	1.13%	0.445
	Maximum energy of collisions	8.71e-11 J	1.34e-10
	Frequency of collisions of maximum energy	0.0181 1/s	0.00474
Liquid-solid mass transfer	Average mass transfer coefficient (approx.)	0.000038 m/s	0.0000375

We can see now that the average turbulent dissipation (specific power) in the production tank with the A310 agitator is very close to the same parameter of the pilot crystallizer. Characteristics of distribuion of solid phase – the max. degree of non-uniformity - are also good enough. However, the local value of energy dissipation around the agitator blades, and accordingly – shear rate and maximum energy of collisions of crystals in this case are much higher than in the pilot tank. It can result in a higher particle destruction and nucleation rate. So, it would be better to keep the Max. local value of turbulent dissipation on about the same level as in the pilot tank. This condition can be satisfied if we replace the A310 agitator with a **Pitch paddle** with the following characteristics:

Diameter = 1000 mm;
Number of blades = 3;
Pitch angle = 45 deg;
Width of blade = 200 mm;

The next steps: select **Pitch paddle** and enter the dimensions of the agitator listed above (Figure 34.

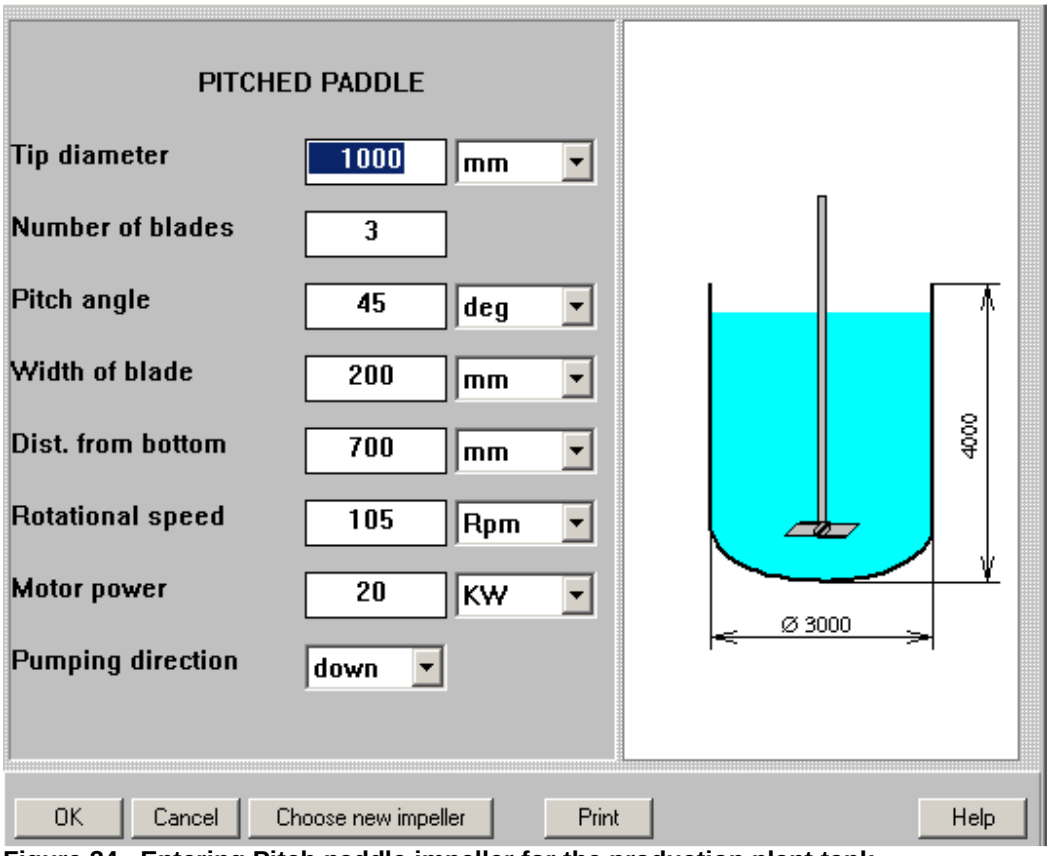


Figure 34. Entering Pitch paddle impeller for the production plant tank.

Now we can perform the calculations in the same order as it has been done for the tank with A310, complete the Table 2 with the new data and compare the calculated parameters of the tank with **Pitch paddle** with the corresponding parameters of the pilot crystallizer (see Table 2b).

Table 2b. Comparison of the pilot and production scale crystallizers.

Menu section	Parameter	Pilot	Production with A310	Production with Pitch paddle
Turbulence	Energy dissipation – maximum value	106 W/kg	204	96.4
	Turbulent shear rate near the impeller blade	9660 1/s	13400	9200
	Relative residence time in zone with maximum dissipation	0.00133	0.000278	0.00127
	Energy dissipation – average value	0.380 W/kg	0.359	0.313
Liquid-solid mixing	Maximum degree of non-uniformity- axial	16.8%	13.0	12.9
	Maximum degree of non-uniformity- radial	1.13%	0.445	0.485
	Maximum energy of collisions	8.71e-11 J	1.34e-10 J	8.15e-11 J
	Frequency of collisions of maximum energy	0.0181 1/s	0.00474 1/s	0.0168 1/s
Liquid-solid mass transfer	Average mass transfer coefficient (approx.)	0.000038 m/s	0.0000375	0.00365

Output tables for **Maximum values of energy dissipation** for the compared mixing conditions are presented also in the Figure 35.

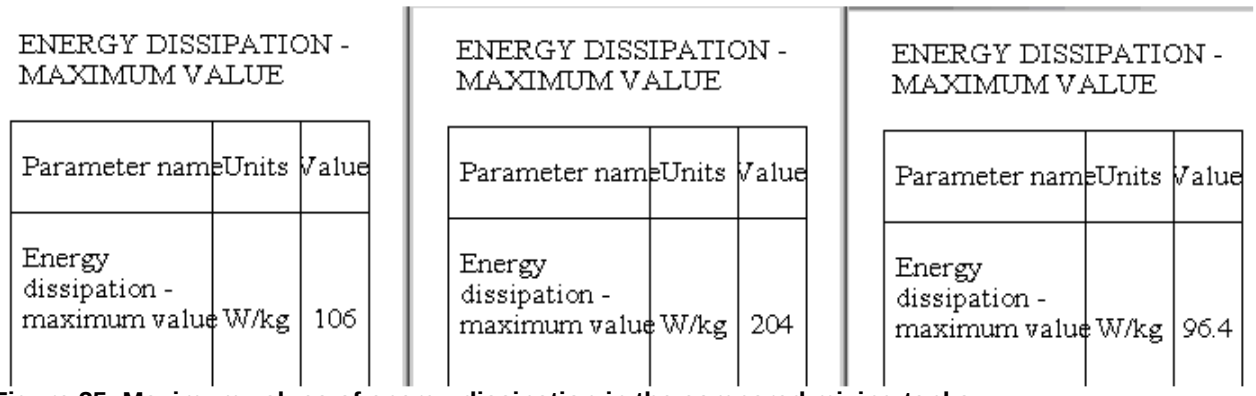


Figure 35. Maximum values of energy dissipation in the compared mixing tanks.

As it follows from the presented results, in the case under discussion mixing with the **Pitch paddle** provides values of the relevant mixing parameters close to the parameters of the pilot crystallizer.