VisiMix TURBULENT

User's Guide

Simulation of Mixing-Related Processes for Chemical Engineers

Mixing in low viscosity fluids
and multiphase systems

Flow pattern, phase distribution,
heat and mass transfer

Jerusalem

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SECTION 1. INTRODUCTION

1.1. Welcome to VisiMix

Welcome to VisiMix, the program intended for chemical, process control, research, and design engineers, as well as for scientists in the field of applied research and modeling of various unit operations dependent on mixing. Students in Chemical Engineering will find it helpful in improving their knowledge on mixing and its influence on reactor performance.

VisiMix provides more than a hundred local and average parameters of a mixing process, including visualizations of flow and mixing patterns and graphs related to the distribution of local parameters (velocities and concentrations) and their change in the course of the mixing.

VisiMix bridges the gap that separates engineering practice from achievements in the field of mathematical simulation. It provides chemical and process engineers with the ability to perform technical calculations based on the results of the most recent experimental research and on mathematical modeling of mixing processes

VisiMix helps:

Production Plant Engineers:

- obtain complete information on the maximum potential and specific features of existing mixing equipment;
- check applicability of equipment for new process applications;
- find solutions to the existing process problems and prevent new problems without equipment change;
- find the inexpensive ways to improve processes and equipment based on the available technical possibilities;

R&D and Pilot Plant Researchers and Engineers:

- perform a more profound analysis of a processes in reactors and other mixing equipment based on the data on the distribution of substances;
- select process regimes based on the desired degree of uniformity and other process requirements;
- reproduce the main features of production plant equipment on a laboratory or pilot plant scale (scaling down) and determine values of the key scaling-up parameters;
- prepare the initial data for selecting or designing production scale mixing equipment;

Design Engineers:

- perform technical calculations;
- choose optimal mixing devices in the range of available technical options;
- prepare the initial data for ordering the equipment;
- analyze, check and compare offers from different equipment suppliers;

Control Engineers:

- simulate transition regimes;
- predict the deviation of the process dynamics from “perfect mixing” conditions;
- obtain the data for developing and programming process control systems;
- define representative positions of sensors.

No special training in either computers or mixing is required to run VisiMix.
The initial data requested by VisiMix - the main dimensions of the mixing tank or reactor, density and viscosity of the media - are either known to you already or can be easily obtained.

NOTE:
If VisiMix does not cover some features of interest to you, such as impellers with variable-angle blades, several baffle kinds in one reactor and so on, contact our technical support department and obtain recommendation on application of VisiMix for this specific case.

1.2. Theoretical Background

VisiMix bridges the gap that separates engineering practice from achievements in the field of mathematical simulation. It provides chemical and process engineers with the ability to perform technical calculations based on the results of the most recent research and on mathematical modeling of mixing processes.
VisiMix is based on the classical approach to the problems of applied hydrodynamics developed by Kolmogoroff, Hinze, and Levich in application to modern deterministic and stochastic mathematical models of mixing phenomena. Theoretical results are used in conjunction with experimental and practical data on unit operations in mixing equipment. The models create a single system, which allows for the performance of several consecutive simulation steps.

At first, the program performs hydrodynamic calculations. This first simulation step serves as a basis for modeling macroscale turbulent transport and microscale characteristics of turbulence in the main areas. These, jointly with the results of hydrodynamic calculations, are used to calculate distributions of shear rates, concentrations of solutes and particles, frequencies of break-up and coalescence of droplets, frequencies and energy of collisions of crystals, and other local process parameters. And finally, average characteristics of mixing in application to various unit operations in stable state and dynamic conditions are calculated.

For instance, defining of the distribution of suspension is based on a few mathematical models and includes:

- Hydrodynamic modeling - calculation of tangential and axial velocity distribution according to the entered initial data on tank design and properties of the suspension;
- Calculation of circumference flow rate;
- Calculation of macroscale turbulent diffusivities in axial and radial directions;
- Calculation of settling velocity of particles as a function of local concentration;

- Calculation of local values of radial velocity of particles in the field of centrifugal force;
- Calculation of local turbulence close to the tank bottom;
- Calculation of up- and down- directed mass flows of solid in vicinity of bottom;
- Calculation of distribution of particles along the vertical axis and radius of the tank.

All mathematical models and methods of calculation have been verified by comparison with experimental data, including the results of measurements in laboratory and production scale tanks and reactors. A detailed description of most mathematical models is given in **Review of Mathematical Models.**

1.3. VisiMix Outputs

VisiMix provides an extensive set of output parameters which enable the user to evaluate the suitability of his mixing equipment, analyze his process, perform scaling-up procedure, etc. In addition to calculating output parameters, VisiMix analyzes the initial data and issues warning messages whenever any of the parameters you have entered is unacceptable for your process from the point of view of safety or efficiency.

The suitability of one or another mixing unit is usually evaluated on the basis of several parameters, such as power consumption, average time of circulation, mass transfer rate, heat transfer rate, etc. VisiMix allows for the calculation of all these values for major designs of tanks and impellers with respect to actual sizes and positions of impeller blades and baffles.

For analysis of processes, trouble-shooting, and scaling-up, more details on mixing are usually required. For these purposes, VisiMix provides an extensive set of average and local parameters and their distributions in the tank volume.

VisiMix output is presented in the form of visualizations, graphs, and tables. The output data is presented mainly in SI units. Conversion tables for various units are given in APPENDIX 1.

1.4. VisiMix TURBULENT Features

User friendly, graphic VisiMix environment lets you:

- Display drawings of the device (apparatus) and its main parts (tank, baffles, impeller) and tables of properties at any calculation stage;
- Change any parameter in your initial data at any calculation stage;
- Display several output windows at once;
- Compare calculated parameters for different sets of initial data (different projects) by simultaneously displaying the appropriate output windows;
- Save equipment designs to create an equipment database, which enables the simulation of various processes on the same equipment without repeated input of equipment data;

- Save the initial data on the equipment and properties of media to create a database of your mixing equipment and processes;
- Use the **Calculate** menu to obtain answers to your questions with respect to various mixing problems;
- Accumulate initial data and the results of the calculations in an HTML file;
- Use **Supplement** menu option for hydrodynamic and heat transfer calculations of tanks with scraper (sweeping-wall) agitators.
- Use program VisiXcel for management of initial data and results of calculations;
- Use a complimentary program VisiMix DI for modeling mixing tanks with multiple different impellers on the shaft.

SECTION 2. SELECTING AND EVALUATION OF MIXING EQUIPMENT.

2.1. Key Scaling-Up Section Parameters for different Unit Operations.

This section will help you to choose **Output Parameters**, which are of a key importance an can be considered as scaling-up parameters for your process. The typical **Unit Operations** corresponding to the main fields of industrial application of mixing equipment are presented in the Table 1. This table includes also the VisiMix output parameters that are recommended for checking applicability of the mixing devices, for process analysis and scaling-up.
Additional information regarding the interpretation, calculation methods, and fields of application of the output data is presented in the following section of the User's Guide and in Help section of the program.

Table 1.1. Hydrodynamics. Turbulence. Single-phase mixing.

Field of equipment application. Unit Operation	Mixer applicability check-up	Key process and scaling-up parameters	
		Menu	**Parameters**
Newtonian and non-Newtonian media. **Hydrodynamics and turbulence – general problems of equipment application.**	**Mixing power** **Vortex formation** **Gas pick-up**	Hydrodynamics	Reynolds mumber
			Average tangential velocity
			Circulation flow rate
			Vortex depth
		Turbulence	Energy dissipation - maximum value
			Energy dissipation in bulk of flow
			Volume of zone of max. dissipation
			Max. local shear rate
2. Single-phase mixing (blending	**Mixing time.** **Max. degree of non-uniformity vs. time**	Hydrodynamics	General flow pattern
			Circulation flow rate
			Distribution of tangential velocity
		Turbulence	Energy dissipation - maximum value
			Energy dissipation in bulk of flow
			Shear rates in different zones
		Single-phase liquid mixing	Macro-mixing time
			Characteristic time of micro-mixing

Table 1.2. Suspension of solid particles. Emulsification (oil-water systems)

Field of equipment application. Unit Operation	Mixer applicability check-up	Key process and scaling-up parameters	
		Menu	**Parameters**
Suspension of solid particles	**Pick-up of solid from bottom.** **Immersion of floating powder (Check gas pick-up)**	Liquid-solid mixing	Complete/incomplete suspension
			Axial distributions of the solid phase
			Radial distributions of the solid phase
			Max. degree of non-uniformity - axial
			Max. degree of non-uniformity - radial
			Max. and min. local concentration of the solid phase
Emulsification (oil-water systems)	**Complete emulsification**	Turbulence	Energy dissipation - maximum value
			Volume of zone of max. dissipation
			Maximum value of shear rate
		Liquid-liquid mixing	Complete/incomplete emulsification
			Mean drop size
			Distribution of drops by diameter
			Kinetics of drop break-up

Table 1.3. Crystallization

Field of equipment application. Unit Operation	Mixer applicability check-up	Key process and scaling-up parameters	
		Menu	**Parameters**
Crystallization	**Pick-up of solid from bottom.** **Maximum and Minimum media and wall temperatures**	Turbulence	Energy dissipation - maximum value
			Shear rate – maximum value
			Relative residence time in zone of max. dissipation
		Single-phase liquid mixing	Macro-mixing time
			Characteristic time of micro-mixing
		Batch reaction/ blending Semi-batch reaction	Max. local concentration vs. time
			Max. difference of concentration vs. time
		Continuous flow reaction	Max. local concentration
			Max. difference of local concentrations

Table 1.3. Crystallization - continue

Field of equipment application. Unit Operation	Mixer applicability check-up	Key process and scaling-up parameters	
		Menu	**Parameters**
Crystallization	**Pick-up of solid from bottom.** **Maximum and Minimum media and wall temperatures**	Turbulence	Turbulent shear rate in zone of maximum dissipation
		Liquid-solid mixing	Complete/incomplete suspension
			Max. degree of non-uniformity - axial
			Max. degree of non-uniformity - radial
			Relative residence time for solid phase
			Maximum energy of collisions
			Frequency of collisions of maximum energy
		Liquid-solid mass transfer	Mass transfer coefficient (average)
		Heat transfer.	Media temperature
			Wall temperature, media side
			Heat transfer rate

Table 1.4. Dissolution. Liquid-liquid extraction. Heterogeneous chemical reaction.

Field of equipment application. Unit Operation	Mixer applicability check-up	Key process and scaling-up parameters	
		Menu	**Parameters**
Dissolution. Liquid-solid chemical reaction.	**Pick-up of solid from bottom.** **Immersion of floating powder (Hydrodynamics, Check gas pick-up)**	Turbulence	Average value of energy dissipation
		Liquid-solid mixing	Complete/incomplete suspension
			Max. degree of non-uniformity - axial
			Max. degree of non-uniformity - radial
			Relative residence time for solid phase
		Liquid-solid mass transfer	Time of complete dissolution
			Concentration of dissolved solid
			Mass transfer rate vs. time
Liquid-liquid extraction Heterogeneous chemical reaction	**Complete emulsification**	Turbulence	Turbulent dissipation – maximum
			Relative residence time in zone of max. dissipation
		Liquid-liquid mixing	Complete/incomplete emulsification
			Sauter mean drop size
			Specific mass transfer area
			Distribution of drop by sizes
			Mean micro-mixing time inside drop
			Micro-mixing time for the disperse phase

Table 1.5. Gas-liquid mixing and mass transfer.

Field of equipment application. Unit Operation	Mixer applicability check-up	Key process and scaling-up parameters	
		Menu	Parameters
Gas dispersion. Absorption. Chemical reaction.	**Distribution of injected gas**	Hydrodynamics	Circulation flow rate
		Turbulence	Energy dissipation in the bulk of volume
			Microscale of turbulence in the bulk of volume
		Gas dispersion and mass transfer	Check gas distribution
			Gas hold-up
			Sauter mean bubble diameter
			Estimated surface aeration rate
			Specific mass transfer area
			Specific mass transfer coefficient
			Specific mass transfer rate
			Depth of gas-liquid media

Table 1.6. Homogeneous chemical reactions.

Field of equipment application. Unit Operation	Mixer applicability check-up	Key process and scaling-up parameters	
		Menu	Parameters
Homogeneous chemical reactions. Batch. Semi-batch.	**By-product formation rate** **By-product quantity** **Maximum / minimum temperature**	Single-phase mixing	Macromixing time
			Characteristic time of micromixing
		Batch reaction	Max. local concentration of reactant B
			By-product formation rate
			By-product quantity
		Semi-batch reaction	Max. local concentration of reactant B
			By-product formation rate
			By-product quantity
		Heat transfer.	Media temperature
			Wall temperature
			Heat transfer rate

Table 1.6. Homogeneous chemical reactions - continued

Field of equipment application. Unit Operation	**Mixer applicability check-up**	**Key process and scaling-up parameters**	
		Menu	**Parameters**
Homogeneous chemical reactions. **Continuous flow reactors**	**Relative deviation from ideal RTD function** **By-product formation rate** **Maximum / minimum temperature**	Hydrodynamics	Circulation flow rate
		Single-phase mixing	Macromixing time
			Characteristic time of micromixing
		Continuous flow dynamics	Response function
			Relative deviation from ideal RTD function
		Continuous flow reaction	Max. difference of Reactant A concentration
			Max. difference of Reactant A concentration
			By-product formation rate
		Heat transfer	Media temperature
			Wall temperature
			Heat transfer rate

Table 1.7. Biotechnology. Fermentation.

Field of equipment application. Unit Operation	**Mixer applicability check-up**	**Key process and scaling-up parameters**	
		Menu	**Parameters**
Fermentation Biotechnology	**Maximum local shear rate** **Distribution of injected gas**	Turbulence	Turbulent shear rate in zone of maximum dissipation
		Gas dispersion and mass transfer	Check gas distribution
			Gas hold-up
			Sauter mean bubble diameter
			Estimated surface aeration rate
			Specific mass transfer area
			Specific mass transfer coefficient
			Specific mass transfer rate

2.2. Selecting Mixing Equipment

VisiMix provides the data for:

- Checking the applicability of available equipment to a given production process;
- Comparing different designs of tanks, baffles, and impellers;
- Selecting the best ways of improving mixing regimes according to your technical possibilities;
- Selecting or designing new mixing units.

Several practical considerations of a general character, which should be taken into account, are listed below.

- At equal values of mixing power, **suspension** is usually more efficient in unbaffled equipment. Impellers with a larger tip diameter are advisable.
- **Mixing of liquid-liquid systems** is usually performed in baffled tanks. Smaller droplets are formed in tanks with small impellers (1/4 of the tank diameter) at relatively high RPM values.
- **Time of drop-breaking** can be reduced by increasing the size and number of the impeller blades, or by using multiple impellers.
- Mixing of multiphase systems with a **light disperse phase** (the density of the disperse phase is lower than the density of the continuous phase) in unbaffled tanks is in most cases inefficient because of the radial separation.
- Most experimental and practical data on **mixing in gas-liquid systems** was obtained for air-water systems in fully baffled tanks with disk turbines. **Gas dispersion in unbaffled tanks is not efficient enough.**
- Using multistage impellers helps increase the critical shaft velocity (see **Mechanical calculations of shafts**) and is sometimes necessary to exclude the shaft vibrations. It also helps accelerate micromixing and reduce micromixing time in **Single-phase** and **Liquid-liquid** mixing. However, the power required for the same degree of macroscale mixing with multistage systems is in most cases higher than for single-stage impellers due to compartmentalization of the flow pattern in the tank.
- **Scraper agitators** are used for mixing of low viscosity media in order to avoid cowering of the tank wall with particles or a film. Such design provides a high heat transfer rate.**The mixing ability of scraped agitators is relatively low.**

While using VisiMix, you will sometimes discover that efficient mixing can be ensured in mixing equipment of several different designs. Final choice of the equipment should be based on the results of mechanical calculations, economic considerations and engineer's common sense.

NOTE: ***If the suitability of your equipment is questionable, VisiMix issues a warning message.***

SECTION 3. PROGRAM INSTALLATION

Installation rules for the ‘stand alone’ and the network version of the program are different. Installation of each program has to be performed accordingly to the Installation instruction that is applied to the program CD.

SECTION 4. STARTING THE PROGRAM

After installing VisiMix, the main VisiMix menu appears on the screen (Figure 1). It has the following structure:

Project
Edit input
Calculate
Supplement
Last menu
Last input table
Window
View
Help

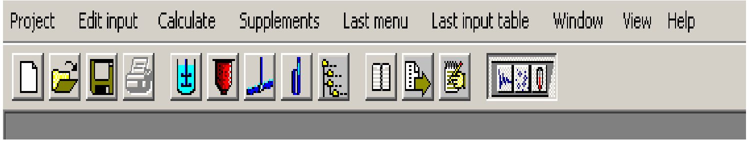


Figure 1.

4.1. Project

VisiMix performs mathematical modeling of processes in relation to a project - a single set of initial data, which includes the types and main dimensions of equipment as well as the physical properties of the media and regime parameters. The project is identified by its name. All output windows corresponding to the same project are displayed in frames of the same color.

To start VisiMix, select **Project**. When the **Project** submenu appears, you have two options: starting a new project or working with one of the projects you have previously stored in the system.

The program enables you to open several projects (up to four) which can be simultaneously displayed on the screen. However, you may modify initial data, create new output windows, or use any other functions only for the current project whose name appears in the text field at the bottom of the screen. To change the current project, use **Project list** option in **View**. The names of four projects with which you last worked, and their locations are displayed at the bottom of the **Project** menu, between **Print** and **Exit** options.

If windows related to several projects are displayed on the screen, you can also change the current project by double-clicking on the colored frame of the window related to the project you now want to become the current one.

4.2. Edit Input

This option gives you access to all input tables related to the Current Project. Use it to selectively modify the initial data, for instance, Average density, Width of blades, or any other parameter by choosing the appropriate submenu item. You may also use **Edit input** to enter initial data, although normally VisiMix automatically requests the required initial data.

NOTE:

When entering initial data through the Edit input option, you may sometimes obtain a different input table from the one you have selected. This means that you must first complete the table invoked by VisiMix, and then the table you have originally selected will be invoked automatically.

The **Edit input** option has the following structure (Figure 2) briefly described below.

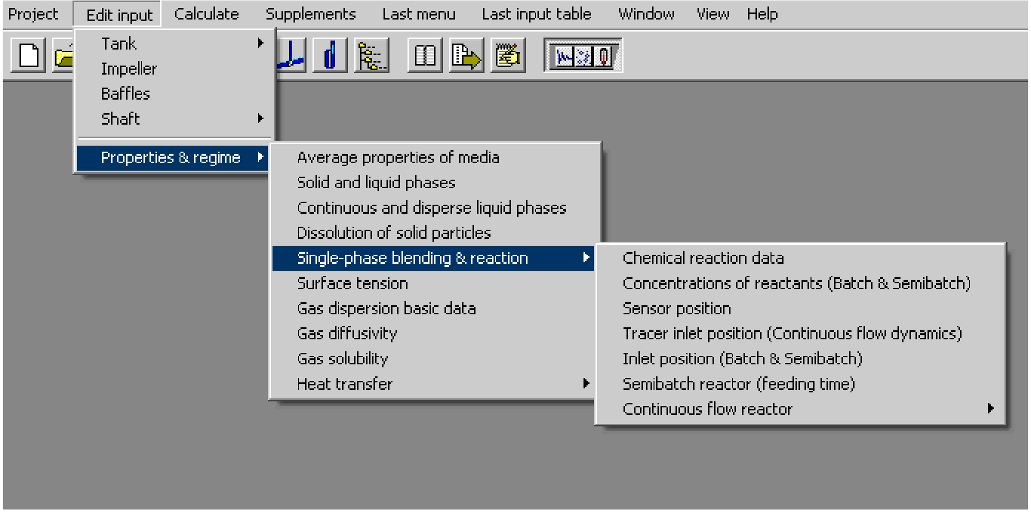


Figure 2.

Tank:

Tank geometry - Main inside dimensions of the tank and volume of media

Tank shell - Tank shell characteristics for heat transfer calculations

Jacket

General characteristics - Main data on various types of jackets, including number of jacket sections, their height, position and connection between the jackets

Specific characteristics - Specific data for each jacket type, i.e. width of conventional jacket and parameters of heat transfer enhancing devices, diameter or half-pipe coil, parameters of embossed/dimpled jackets.

Impeller: Characteristics and dimensions of the impeller.

Baffles: Type, number, position and dimensions of baffles.

Shaft:

Shaft design -Shaft type and dimensions.

Shaft material and impeller mass - Properties of the shaft materials and impeller mass.

Properties & Regime:

Average properties of media - Average density and viscosity, or rheological parameters for non-Newtonian media, used for hydrodynamic calculations.

Solid and liquid phases - Properties of phases used for modeling of mixing in solid-liquid systems.

Continuous and disperse liquid phases - Properties of immiscible liquids required for modeling mixing in liquid-liquid systems.

Dissolution of solid particles - Specific properties of substances related to mass transfer: solubility, diffusivity. Mass transfer regime parameters.

Single-phase blending & reaction:

Chemical reaction data Data for simulation of isothermal 2nd order chemical reaction (for both main and side reactions).

Concentrations of reactants (Batch & Semibatch) – initial concentrations of reactants brfore the reaction.

Sensor position – point for concentration measurement, actual or imagined.

Tracer inlet position (Continuous flow dynamics)

Inlet position (Batch & Semibatch) – point of the reactant B injection.

Semibatch reactor (feeding time) - Feeding time for adding of reactant B, which is used for simulation of a Semibatch reactor only.

Continuous flow reactor:

Inlet flows. Inlet and outlet positions.

Concentrations of reactants in inlet flows.

Heat transfer:

Heating vaporous agent - Heating steam pressure or data for another condensing heating agent.

Heating/cooling liquid agent - Liquid heat transfer agent, its flow rate and initial temperature.

Heat transfer properties of the media - Physical properties of the media required for heat transfer calculations.

Chemical reaction data & regime - Kinetic constants for non-isothermal reaction, heat effect, process temperature range. **Continuous flow** - Data used for simulation of temperature regime of continuous flow tanks and reactors only - flow rate of media, temperature and concentration of reactants in the inlet flow, etc.
tanks and reactors only - initial temperature and concentration of reactants, feeding time, etc.

Batch -Data used for simulation of temperature regime of Batch tanks and reactors only - initial temperature and concentration of reactants, etc.

Fixed temperature regime - Media temperature.

Gas dispersion basic data - a minimum set of data required for any Gas-Liquid calculations: volume flow rate of gas, surface tension, operating conditions (fixed liquid volume/liquid level)

Gas diffusivity - molecular diffusivity of the gaseous component in the liquid which is necessary for mass transfer calculations

Gas solubility - solubility of the gaseous component of the liquid, which cannot be calculated and must be entered from the reference or practical data for each individual gas-liquid couple.

4.3. Calculate

Use this option to perform the calculations. The **Calculate** submenu provides access to modeling in relation to all mixing problems and output parameters.

4.4. Supplement

This option allows to enter data and to perform calculations for tanks with scraper (sweeping-wall) agitators. As it follows from the Figure 3, for this agitator type the program provides calculations of hydrodynamics and heat transfer only.

4.5. Last Menu

This convenient option enables you to directly invoke the **Calculate** submenu with which you last worked.

Example:
You have clicked on **Mixing power** in the **Hydrodynamics** submenu and obtained a corresponding output. In order to obtain another output parameter, for instance, **Vortex depth,** you do not need to return to the **Calculate** menu. Simply click on **Last menu - Vortex depth** to obtain your output**.**

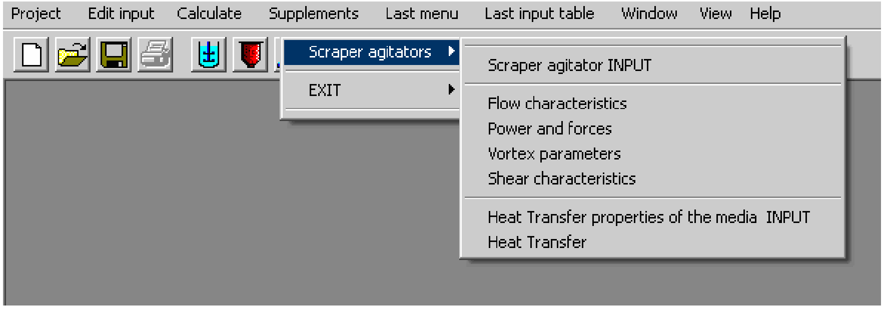


Figure 3.

4.6. Last Input Table

This is another shortcut, which enables you to directly invoke the input table with which you last worked. For example, if you want to compare heat transfer rates and select the best vaporous heat transfer agent, you can change the input after each calculation by selecting **Last input table** only, without going through the long procedure of addressing **Edit input- Properties & Regime - Heat Transfer**. This option is activated after you have first accessed an input table through the **Edit input** option or the quick access buttons in the upper screen bar.

4.7. Window

This option functions the same way it does in Microsoft Windows.

4.8. View

This option contains the following functions:

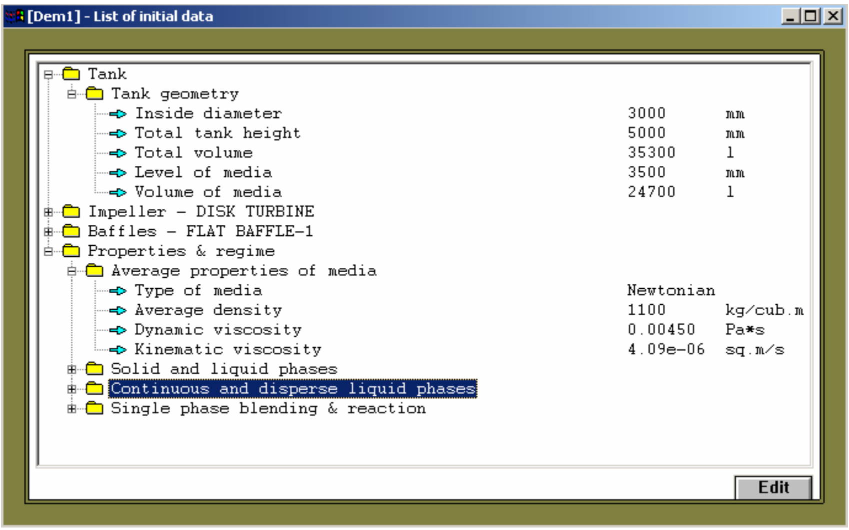
Toolbars
Initial data explorer
Project list
Drawing of apparatus

4.8.1. Toolbars

This option allows you to display or remove the main toolbar located in the upper screen bar, and the **Calculate** toolbar located in the right screen bar. To remove or display the **Calculate** toolbar you can also use a quick access button in the main toolbar.

4.8.2. Initial data explorer

This option (Figure 4) shows a list of initial data for the current project, including equipment data (tank, impeller, shaft and baffle), and properties & regime parameters (see the description of the **Edit input** option above). This option is also accessible from a quick access button in the upper screen bar. To modify any of the initial data using the initial data explorer, select the required item, and press the **Edit** button at the bottom of the screen. The appropriate input screen will be invoked.



```
Tank
  Tank geometry
    Inside diameter                         3000       mm
    Total tank height                       5000       mm
    Total volume                            35300      l
    Level of media                          3500       mm
    Volume of media                         24700      l
Impeller - DISK TURBINE
Baffles - FLAT BAFFLE-1
Properties & regime
  Average properties of media
    Type of media                           Newtonian
    Average density                         1100       kg/cub.m
    Dynamic viscosity                       0.00450    Pa*s
    Kinematic viscosity                     4.09e-06   sq.m/s
  Solid and liquid phases
  Continuous and disperse liquid phases
  Single phase blending & reaction
```

Figure 4.

4.8.3. Project list

This option invokes the Project list dialogue, which contains a list of opened projects. In this dialogue, you can choose or change the current project. The name of the current project appears in the text field at the bottom of the screen**.** This option is also accessible from a quick access button in the upper screen bar.

4.8.4. Drawing of apparatus

This option shows the diagram of the mixing system for the current project, with main dimensions. This diagram automatically appears on the screen after all basic initial data for a new project has been entered, or when an existing project is opened. It is also accessible from a quick access button in the upper screen bar.

4.9. Help

This option functions the same way it does in Microsoft Windows. Press **F1** to invoke the **Help** section corresponding to the active window.

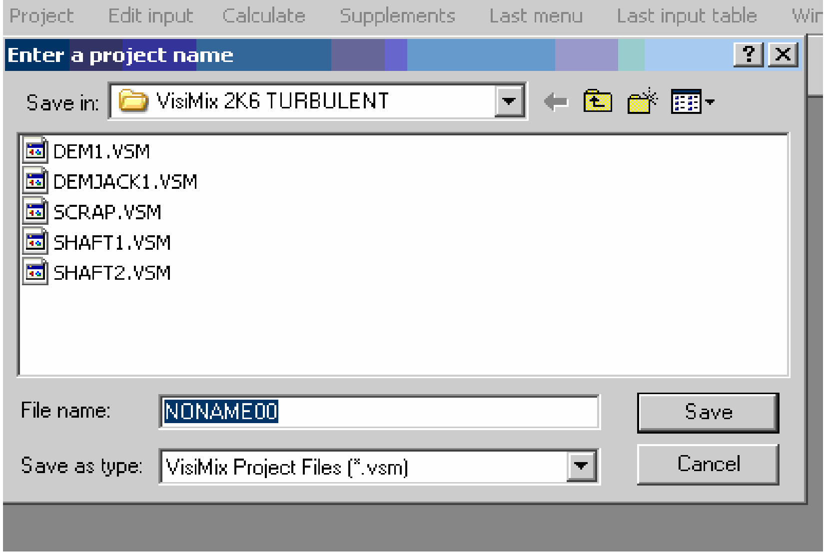
SECTION 5. STARTING OR OPENING A PROJECT.

Select **Project**. The following submenu appears:
New
Open
Close
Clone
Project comments
Save
Save as
Report
Print
[Recent projects]
Exit

5.1. New

To start a new project:

1. Select **New** from the **Project** menu.
2. When the new project dialogue appears (Figure 5), enter a project name in the name field, then click **Save**.



File name: NONAME00

Save as type: VisiMix Project Files (*.vsm)

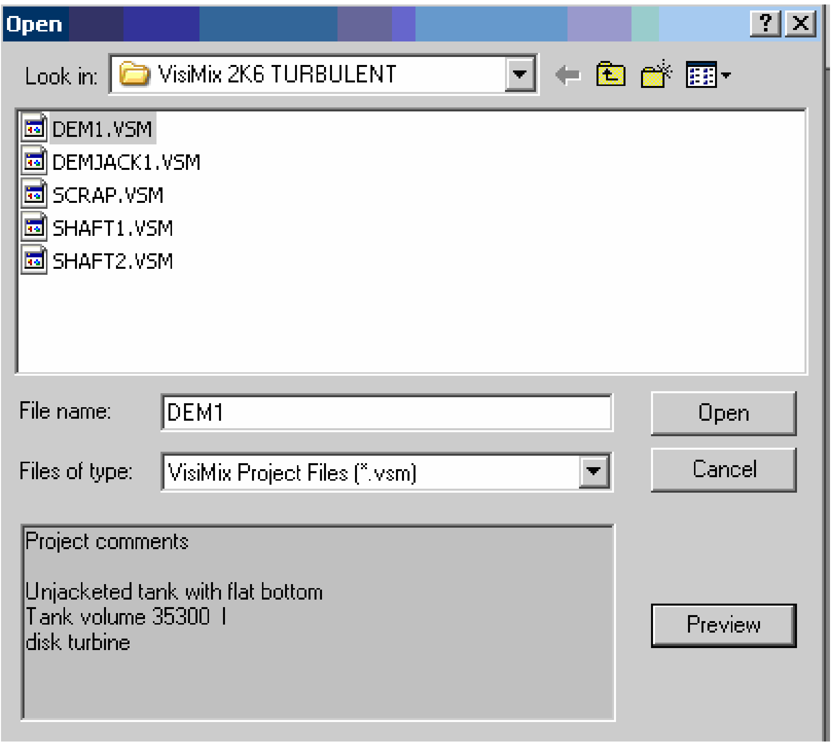
Figure 5.

This option is also accessible from a quick access button in the upper screen bar.

5.2. Open

To open an existing project:
1. Select **Open** from the **Project** menu. The **Open** dialogue appears (Figure 6).
The text box at the bottom of the screen displays basic information about the project you have selected (tank type, volume of the media, impeller), and your comments to the project if any have been made.

Press **Preview** button to display detailed information about the selected project (tank, impeller, baffle, and media properties), and the diagram of the mixing system (Figure 7). Press **Close** button at the bottom to exit the **Preview** dialogue.



Look in: VisiMix 2K6 TURBULENT

DEM1.VSM
DEMJACK1.VSM
SCRAP.VSM
SHAFT1.VSM
SHAFT2.VSM

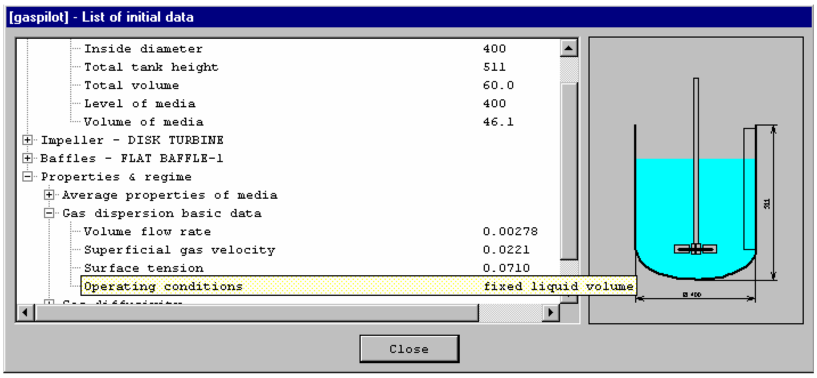
File name: DEM1

Files of type: VisiMix Project Files (*.vsm)

Project comments

Unjacketed tank with flat bottom
Tank volume 35300 l
disk turbine

Figure 6.



```
        Inside diameter                  400
        Total tank height                511
        Total volume                     60.0
        Level of media                   400
        Volume of media                  46.1
⊞ Impeller - DISK TURBINE
⊞ Baffles - FLAT BAFFLE-1
⊟ Properties & regime
    ⊞ Average properties of media
    ⊟ Gas dispersion basic data
        Volume flow rate                 0.00278
        Superficial gas velocity         0.0221
        Surface tension                  0.0710
        Operating conditions             fixed liquid volume
```

Figure 7.

2. From the file browser screen select the desired project and click **Open.** The system displays a diagram of the apparatus and its main dimensions. Use the **Edit input** option, **Initial data explorer** or the quick access buttons in the upper screen bar to check and modify initial data for your equipment (Tank, Baffles and Impeller). For media properties and regime characteristics, use **Edit input** option or **Initial data explorer** only (Properties & Regime).

The **Open** option is also accessible from a quick access button in the upper screen bar.

You can also open any of the four projects with which you last worked from a list of recent projects displayed at the bottom of the **Project** menu above the **Exit** option.

5.3. Close

Use this option to close and save the current project.

5.4. Clone

Use this option to create up to four copies of you current project. It serves as a convenient tool for comparing different variants of the same basic project. This option is also accessible from a quick access button in the upper screen bar.

5.5. Project comments

Use this option to create or modify your comments to the project. This option is also accessible from a quick access button in the upper screen bar.

5.6. Save

Use this option to save all initial data for the current project. This option is also accessible from a quick access button in the upper screen bar.

5.7. Save as

Use this option to save the current project under a new name.

5.8. Report

Use this option to accumulate the initial data and calculated results in a file of standard HTML format.

Selecting **Report** at any stage of working on a current project invokes a submenu, which is identical to the **Calculate** submenu (Figure 8).

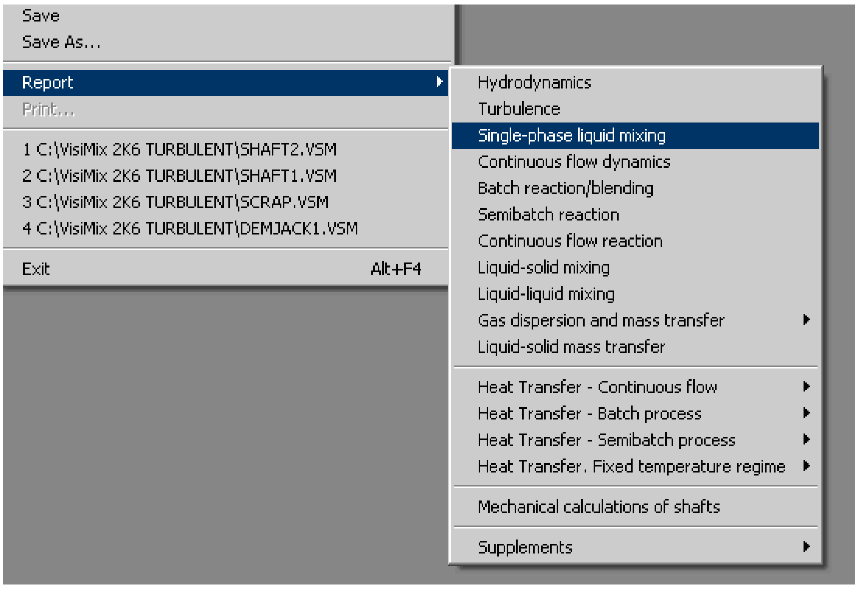
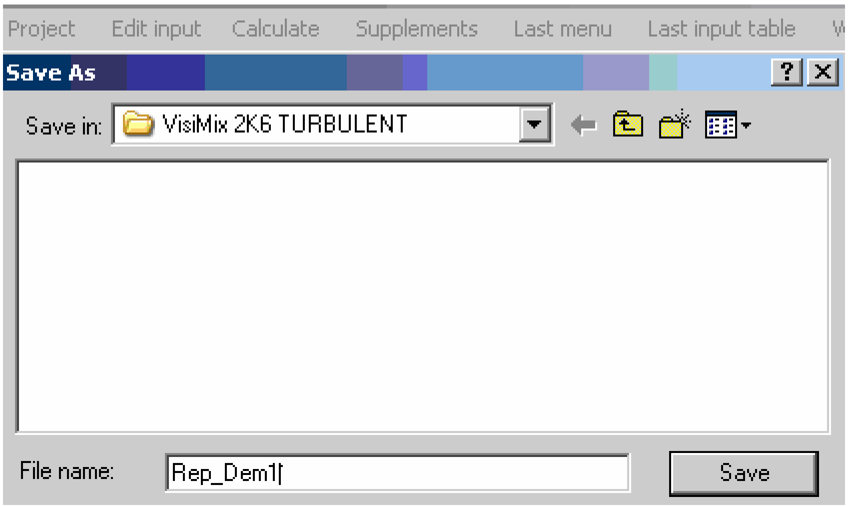


Figure 8.

Choose any item you are interested in, and supply additional data if requested by VisiMix. When the required initial data is entered, VisiMix asks you to enter a name for the report.

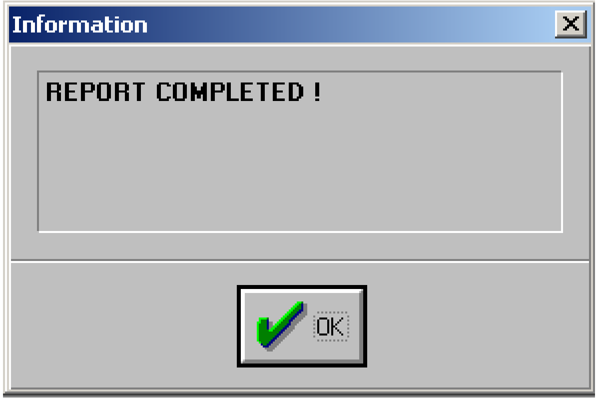
Enter the report name (Figure 9), and VisiMix will create a report containing relevant initial data and the results of the calculations.



File name: Rep_Dem1

Figure 9.

On completing the report, VisiMix issues an appropriate message (Figure 10).



REPORT COMPLETED !

Figure 10.

You may create one or more reports for your project.
The report is formed as a file with a **.htm** extension, and you may open, edit and print this file from Microsoft Internet Explorer or Microsoft Word (Microsoft Office 97 or higher). To work with your report files in Microsoft Word, make sure that the HTML converter option is on.
The report files are opened as usual files with **.htm** extension.

5.9. Print

Use this option to print the content of the active output window - the window, which always has a blue caption. This option is also accessible through a quick access button in the right part of the screen.

Various groups of initial data (tank, impeller, baffles, average properties of media, and so on) are printed from the corresponding input data tables.

Each print-out also includes the complete information on the project and directory names.

5.10. Exit

Use this option to close opened projects and quit VisiMix.

After you enter the name of a new project and click OK, VisiMix requests basic initial data required for all calculations by invoking the appropriate input tables. Supplying this data allows the program to start the calculations. You can use the **Calculate** function before all initial data is entered, but VisiMix will ask you to supply all parameter values first.

Whenever you choose an item for simulation from the **Calculate** submenu, VisiMix will request additional data required for modeling or calculating the selected parameter. You do not need to enter any additional data unless VisiMix requests it. The data you have entered is stored in the system, and when addressing any further parameters of the output submenus, you will be asked to enter only data that is required for modeling the selected parameter and which has not been entered previously.

You may enter any input parameter in SI or US customary and commonly used units.

Use the **Edit input** option, **Initial data explorer**, or **Last input table** option to selectively modify your initial data.

VisiMix verifies the input. If your input contains inapplicable symbols, e.g. characters or punctuation marks instead of numbers, VisiMix issues a message indicating that one of the input values is incorrect. In this case you must click **OK** and correct the error. If your input is outside reasonable limits, contradicts previously entered data, or is beyond VisiMix calculation range, VisiMix modifies the input, offering the nearest acceptable value to the one entered, and issues an appropriate message when necessary. In this case you should check the data before exiting the input table.

6.1. Tank

After you enter the name of a new project and click **OK,** the **Tank types** graphic selection of tanks appears, differing by **bottom type** (flat, conic or elliptical) and **type of a heat transfer device** (conventional, half-pipe coil, embossed/ dimpled jacket, or no heat transfer device) (Figure 11).

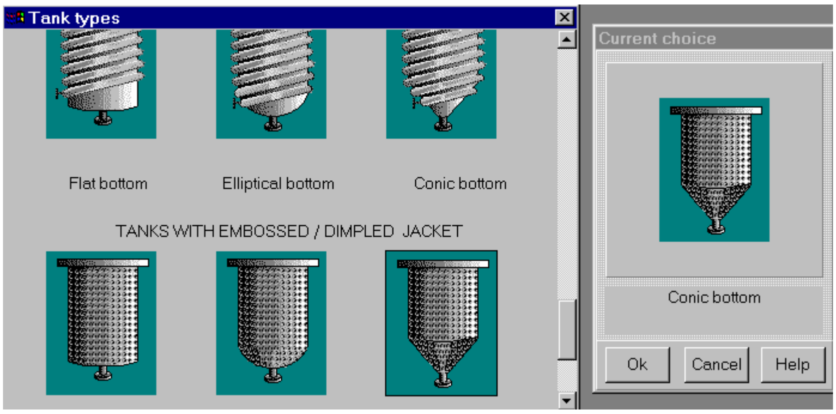


Figure 11.

The **jacket** may consist of one section, or two sections connected **in series** or **in parallel**. Choose a tank by clicking anywhere inside the selected drawing. The tank you have selected will appear in the **current choice** window on the right. Click **OK** to confirm your choice**.**

NOTE:
If you do not plan to perform heat transfer calculations in the current project, do not select a jacketed tank, even if your tank has a heat transfer device. Select an equivalent unjacketed tank instead. If you select a tank with a heat transfer device, you will be asked to supply all its parameters.

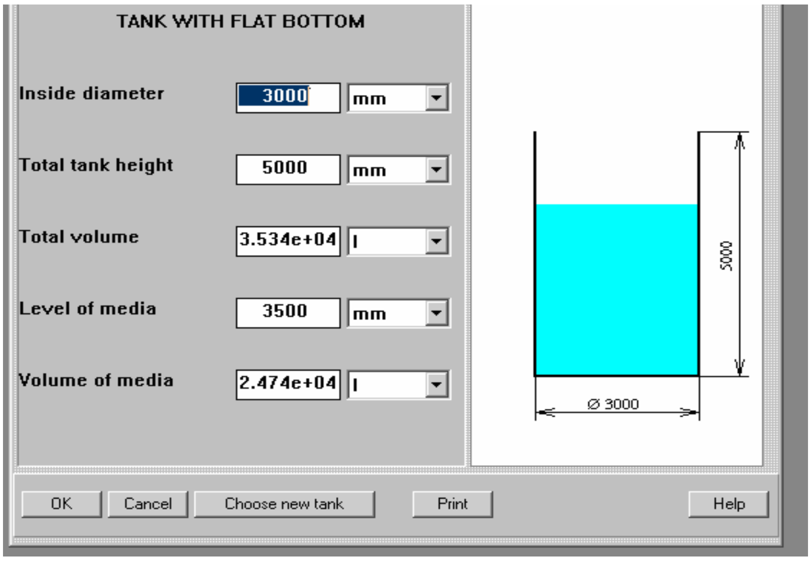
When the scheme of the selected tank appears, supply the requested values of tank parameters by completing the table of dimensions.

NOTE:
The Total tank height is measured from the lowest point of the bottom for bottoms other than flat to the upper edge of the tank, tank head not included.

6.1.1. Tank with flat bottom

Supply the internal dimensions of the selected flat-bottomed tank (Figure 12). Enter the **Inside diameter** and either the **Total tank height,** or **Total volume**, and the second parameter will be entered automatically. The same applies to the **Level of media** and **Volume of media.** After the table has been completed, click anywhere on the field of the window, and the diagram on the screen will change to reflect your input. Click **OK** to confirm your input, and use the **Choose new tank** button at the bottom of the screen to change the tank type. The TANK TYPES screen will then be displayed.

NOTE:
In modeling Heat transfer Semibatch process, the Volume of media is understood as an initial value. In calculations of Gas-Liquid Mixing, the Level of media can be considered as the initial liquid level before gas injection, or as the final level of the gas-liquid mixture in the tank. The last case is more typical for continuous flow gas-liquid reactors.


TANK WITH FLAT BOTTOM

Inside diameter 3000 mm
Total tank height 5000 mm
Total volume 3.534e+04 l
Level of media 3500 mm
Volume of media 2.474e+04 l

Figure 12.

6.1.2. Tank with elliptical bottom

Supply the internal dimensions of the selected tank with an elliptical bottom. This option may also be used for calculating tanks with a spherical bottom, as the influence of the difference in geometry proves to be insignificant for the process modeling. Enter the **Inside diameter** and either the **Total tank height,** or **Total volume**, and the other parameter will be entered automatically. The same applies to the **Level of media** and **Volume of media.** After the table has been completed, click anywhere on the field of the window, and the diagram on the screen will change to reflect your input. Click OK to confirm your input, and use the **Choose New Tank** button at the bottom of the screen to change the tank type. The TANK TYPES screen will then be displayed.
NOTE:
In modeling Heat transfer Semibatch process, the Volume of media is understood as an initial value. In calculations of Gas-Liquid Mixing, the Level of media can be considered as the initial liquid level before gas injection, or as the final level of the gas-liquid mixture in the tank.

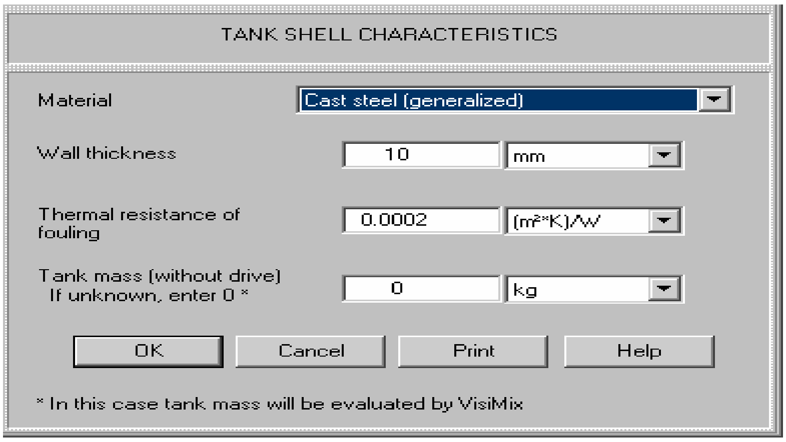
6.1.3. Tank with conical bottom

Supply the internal dimensions of the selected tank with a conical bottom. The **Cone angle** is usually 45-60 degrees. The maximum **Height of cone** is controlled by VisiMix as a function of the **Inside diameter** and the **Cone angle.**

Enter the **Inside diameter**, cone dimensions, and either the **Height of Cylindrical Part,** or **Total volume**, and the other parameter will be entered automatically. The same applies to the **Level of media** and **Volume of media.** After the table has been completed, click anywhere on the field of the window, and the diagram on the screen will change to reflect your input. Click OK to confirm your input, and use the **Choose New Tank** button at the bottom of the screen to change the tank type. The TANK TYPES screen will then be displayed.
NOTE:
In modeling Heat transfer Semibatch process, the Volume of media is understood as an initial value. In calculations of Gas-Liquid Mixing, the Level of media can be considered as the initial liquid level before gas injection, or as the final level of the gas-liquid mixture in the tank.

6.1.4. Tank shell characteristics

You will be asked to fill in this table (Figure 13) if you have selected a tank with a heat transfer device (**HTD**) for the current project.


TANK SHELL CHARACTERISTICS

Material: Cast steel (generalized)

Wall thickness: 10 mm

Thermal resistance of fouling: 0.0002 (m²*K)/W

Tank mass (without drive)
If unknown, enter 0 *: 0 kg

* In this case tank mass will be evaluated by VisiMix

Figure 13.

Material. Select the desired tank material. All the required data for the selected material will be supplied by the program.

Wall thickness. This parameter is required for calculating the wall thermal resistance. If you do not know the exact figure, enter an approximate estimate; for steel tanks it is usually 5-9 mm. You may not enter a wall thickness lower than 1.5 mm.

Thermal resistance of fouling. Fouling of the heat transfer area may occur both on the jacket and on the media side of the tank wall. Thermal resistance of fouling depends on the kind of heat transfer agent (HTA) and the properties of the media, and is estimated according to available practical data. Some typical values for deposit layers not exceeding a thickness of 0.5 mm on the surface of stainless steel plates are given in Help section and in the Table in APPENDIX 2. Enter the estimated value, or zero if there is no fouling. In the case of fouling on both sides of the wall, enter the sum of the estimated values of the corresponding thermal resistance values for each side.

Tank mass. Enter the **Tank mass** value, which is necessary for simulation of heating/cooling dynamics. The **Tank mass** must include the mass of the head, HTD, baffles, shaft and impeller, and should not include the mass of the impeller's drive. It is always preferable to enter the mass value, which has been calculated by the tank designer and appears in the tank technical drawings. If this value is not known, enter "0". In this case the program will calculate the tank mass based on the tank dimensions and material. However, this calculation does not take into account any additional parts of the tank device, and is therefore approximate.

6.1.5. Tank heat transfer general data.

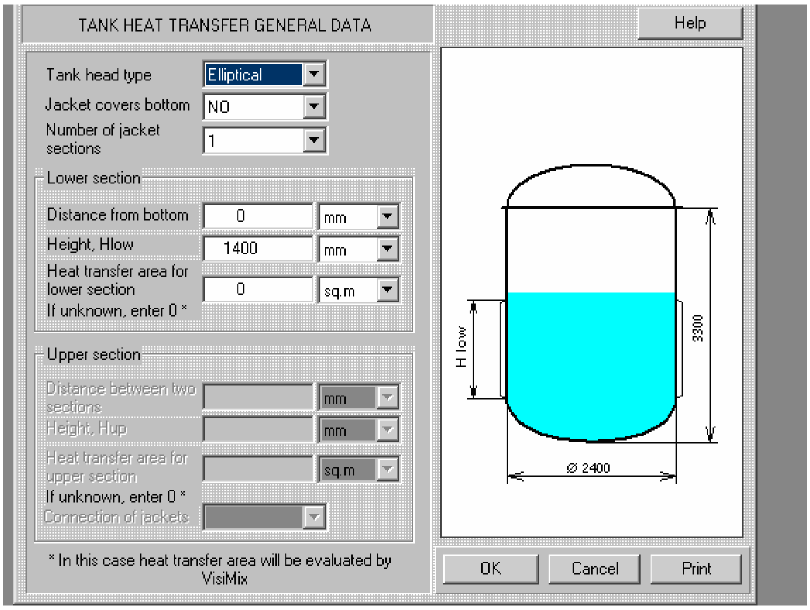
You will be asked to fill in this table (Figure 14) if you have selected a tank with a heat transfer device (HTD) for the current project.

A diagram of a jacketed tank will appear, according to the selected Tank type and dimensions.

Tank head type. Enter tank head type (flat, elliptical), or “absent” for an open tank.

Jacket covers bottom. If you choose **YES,** the heat transfer area of the bottom will be assumed to equal 2/3 of its total area. In most cases, heat transfer area of the bottom part of the HTD constitutes only a small part of the entire heat transfer area.

Number of jacket sections. You may perform calculations for jackets consisting of one or two separate sections. If you choose "1", the program will assume your tank has lower jacket only. In this case, parameters relating to the upper jacket section will appear in inactive script.


TANK HEAT TRANSFER GENERAL DATA

Tank head type: Elliptical
Jacket covers bottom: NO
Number of jacket sections: 1

Lower section
Distance from bottom: 0 mm
Height, Hlow: 1400 mm
Heat transfer area for lower section If unknown, enter 0 *: 0 sq.m

Upper section
Distance between two sections: mm
Height, Hup: mm
Heat transfer area for upper section If unknown, enter 0 *: sq.m
Connection of jackets:

* In this case heat transfer area will be evaluated by VisiMix

Figure 14.

Distance from bottom. For tanks with elliptical or conical bottom, enter the distance from the edge of the shell cylindrical part.

Heat transfer area. Enter the exact values of the HT area for each jacket section, if known. If not, enter zero, and the program will calculate the HT area according to your input.

Connection of jackets. For a **2-section jacket**, specify if the sections are connected **in series,** or **in parallel**. For liquid heat transfer agents (LA), VisiMix assumes that the inlet tube is located in the lower cross-section, and the outlet - in the upper cross-section of each jacket section. The jacket sections are assumed to be connected **in series,** if the **Lower section** outlet is connected to the **Upper section** inlet. For condensing vaporous heat transfer agents (VA), the inlet tube is supposed to be located in the upper cross-section, and the outlet - in the lower cross-section of each jacket section. The jacket sections are assumed to be connected **in series,** if the **Upper section** outlet is connected to the **Lower section** inlet.

6.1.6. Tank jacket.Specific characteristics.

Half-pipe coil jacket. Specific characteristics.

You will be asked to fill in this table (Figure 15) after you have selected a tank with a Half-pipe coil HTD and completed the TANK HEAT TRANSFER GENERAL DATA input table. The entire table appears in active script if a 2-section jacket has been selected. For a single-section jacket, only the **Lower section** boxes are active.

Pipe diameter. Enter the inside diameter of the Half-pipe coil jacket.

Distance between coils. Enter the distance between the axes of the adjacent half-pipe turns as shown in the diagram.

Number of starts. Enter the number of starts of the Half-pipe coil (1 or more, according to the tank design).

NOTE:
If you have a 2-section jacket and attempt to exit the table without entering data for both jacket sections, VisiMix issues an appropriate message.

Conventional jacket. Specific characteristics.

You will be asked to fill in this table (Figure 16) after you have selected a tank with a conventional jacket and completed the TANK HEAT TRANSFER GENERAL DATA input table.

The entire table appears in active script if a 2-section jacket has been selected. For a single-section jacket, only the **Lower section** boxes are active.

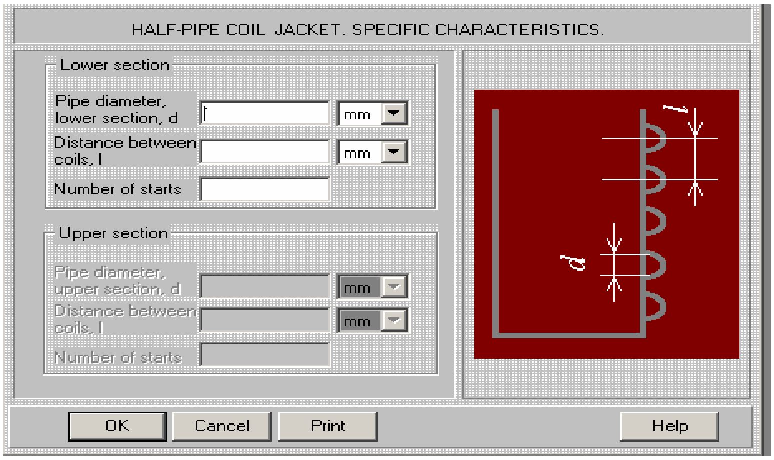
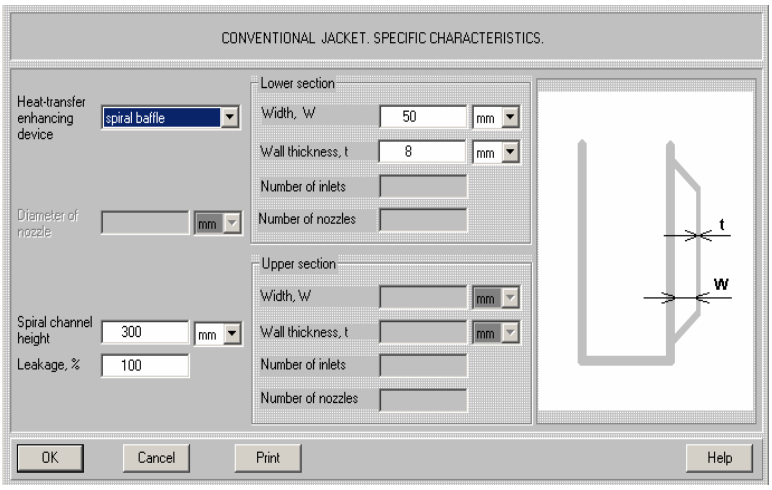


Figure 15.



CONVENTIONAL JACKET. SPECIFIC CHARACTERISTICS.

Heat-transfer enhancing device: spiral baffle

Spiral channel height: 300 mm

Leakage, %: 100

Lower section

Width, W: 50 mm

Wall thickness, t: 8 mm

Figure 16.

Width, W. Enter the width of the channel inside the jacket, i.e. half of the difference between the inside diameter of the jacket and the outside diameter of the tank.

Wall thickness, t. Enter the thickness of the jacket wall.
In addition to the jacket dimensions, the parameters of devices used for improving the jacket heat transfer, such as agitation nozzles and spiral baffles, are entered in this table.

Heat-transfer enhancing device. Select “agitation nozzles” or “spiral baffle” for an appropriate heat-transfer enhancing device. Select “absent” if your jacket has no heat-transfer enhancing device.

Agitation nozzles are mainly used in glass-lined equipment. Their main effect is to impose a spiral flow pattern tangential to the jacket wall by momentum exchange between the high-velocity tangential stream leaving the nozzle and the jacket fluid. This momentum exchange results in “swirl velocities” in the range of 0.3-1.2 m/s, which is high enough to cause turbulent flow [Donald H. Bollinger, Assessing Heat Transfer in Process Vessel Jackets, *Chemical Engineering*, September 20, 1982, pp. 95-100]. VisiMix takes into account both agitation nozzles, which create a spiral tangential flow, and additional inlets that may be located on the jacket surface.

NOTE: ***The flow rate through all inlets is assumed to be the same. va***

The following parameters are entered for the jackets with agitation nozzles:

Diameter of nozzle. Enter the throat diameter of the agitation nozzle.

Number of inlets. Enter the total number of inlets for the jacket, including agitation nozzles.

Number of nozzles. Enter the number of agitation nozzles in the jacket (2-3 agitation nozzles are recommended).

Agitation nozzles produce jacket heat-transfer coefficients two or three times higher than those in conventional jackets without nozzles, however, more pumping energy is required to overcome nozzle pressure drop.

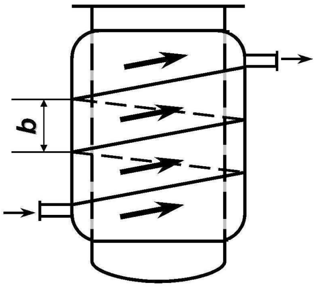
A **spiral baffle** consists of a metal strip spirally wound around a vessel wall from jacket entrance to exit. This strip directs the flow in a spiral path to obtain fluid velocities, typically in the range of 0.3-1.2 m/s. The baffle is manufactured in such a way that a gap is often left between the baffle and the jacket wall. This gap is a second path for the fluid flow from the jacket inlet to outlet, perpendicular to the desired path along the baffle. The fluid that leaks, i. e. bypasses the spiral baffle through this gap, does not contribute directly to heat transfer at the vessel wall. In general, leakage flow amounts to one-third to one-half of the total flow circulated to a spirally baffled jacket.

Compared to agitation nozzles, spiral baffles require a higher flow rate of the heat transfer agent, but result in much less of the pressure drop, to ensure the same heat-transfer rates. Spirally baffled jackets, therefore, require only a part of the energy (typically, not more than about 40%) needed by jackets with agitation nozzles.

The following parameters are entered for the spiral baffle:

Spiral channel height, b. Enter the distance between the adjacent spiral turns for the spiral baffle (see the diagram below).

Leakage, %. Enter the estimated part of the heat transfer fluid that bypasses the spiral baffle through the gap between the baffle and the jacket wall.



Conventional jacket with spiral baffling

Embossed and dimpled jackets. Specific characteristics.

You will be asked to fill this table (Figure 17) after you have selected a tank with embossed or dimpled jacket and completed TANK HEAT TRANSFER GENERAL DATA input table. Embossed and dimpled jackets ensure better heat exchange and higher efficiency than conventional jackets. Tanks with **embossed** or **dimpled** jackets are manufactured using a special double-layer metal plate, which is preliminarily embossed or dimpled.

Plate type. Enter the jacket type – embossed or dimpled.

Embossed. This type of plate is made by (1) contact welding of two metal sheets of different thickness so that welded spots are formed at regular spacing from each other and (2) by hydraulic or pneumatic pressure, so that the thicker plate remains flat, and the thinner one is inflated. As a result, a channel of a variable cross-section is formed. The maximum height of the channel is in the range of 3-15 mm. Any material compatible with resistance welding may be used.

Dimpled: fabricated by welding a pre-deformed metal sheet to a flat plate, so as to obtain a channel of a variable cross-section between the plates, the maximum channel height usually varying from 3 to 15 mm, as for embossed plates.

A diagram corresponding to your choice appears on the screen. Enter the dimensions as shown in the diagram:

Plate thickness, t.
Pillow height, w.
Spot diameter, d.
Spot spacing, l.

All geometrically possible values are allowed.

EMBOSSED / DIMPLED JACKET. SPECIFIC CHARACTERISTICS.

Plate type: embossed
Plate thickness, t: 8 mm
Pillow height, w: 10 mm
Spot diameter, d: 13.33 mm
Spot spacing, l: 40 mm
Flow obstruction factor, lower section: 1
Flow obstruction factor, upper section:

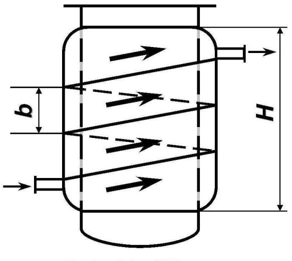
Figure 17.

Embossed and dimpled jackets are sometimes equipped with spiral, horizontal, or vertical baffles for further intensification of the heat transfer. In this case, you are requested to enter an additional parameter, **Flow obstruction factor, FOF** which characterizes the decrease in the flow cross-section due to the heat-transfer enhancing device.

If your embossed/dimpled jacket has no heat-transfer enhancing device, enter "**1**" for the **Flow obstruction factor**.

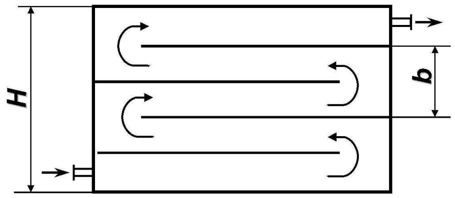
Flow obstruction factor, FOF. Enter the ratio of the flow area in the baffled channel to the unbaffled flow area. This coefficient shows the narrowing of the channel and, accordingly, the increase in the flow velocity.

For the spiral baffling of the jacket shown in the diagram below,
FOF = H/b.



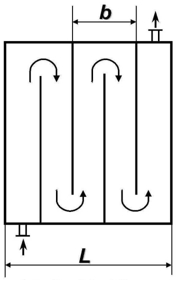
Embossed/dimpled jacket with spiral baffling

For the horizontal baffling shown in the diagram below, **FOF = 2H/b**.



Embossed/dimpled jacket with horizontal baffling

For the vertical baffling shown in the diagram below, **FOF = 2L/b**.



Embossed/dimpled jacket with vertical baffling

In the case of series connection of the internal heat transfer devices,
FOF = n, where **n** is number of plates constituting the heat-transfer device.

In all other cases, the **FOF** *value must be selected empirically, based on general engineering considerations.*

6.2. Baffles

The procedure for selecting the baffle type and entering baffle data is similar to the one used for tanks.
VisiMix selection of baffles is shown in Figure 18.

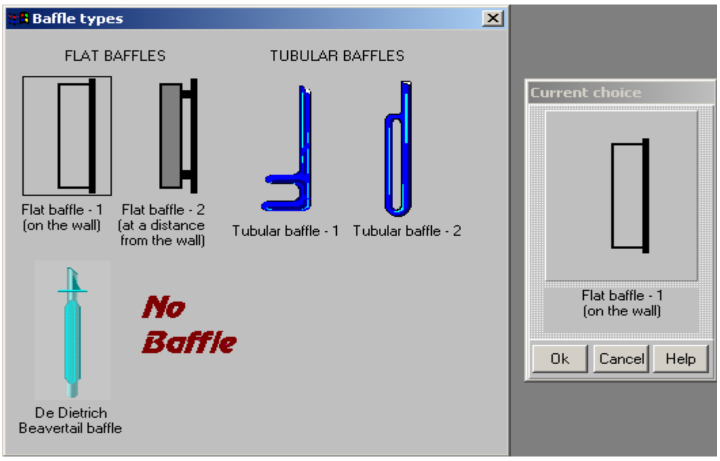
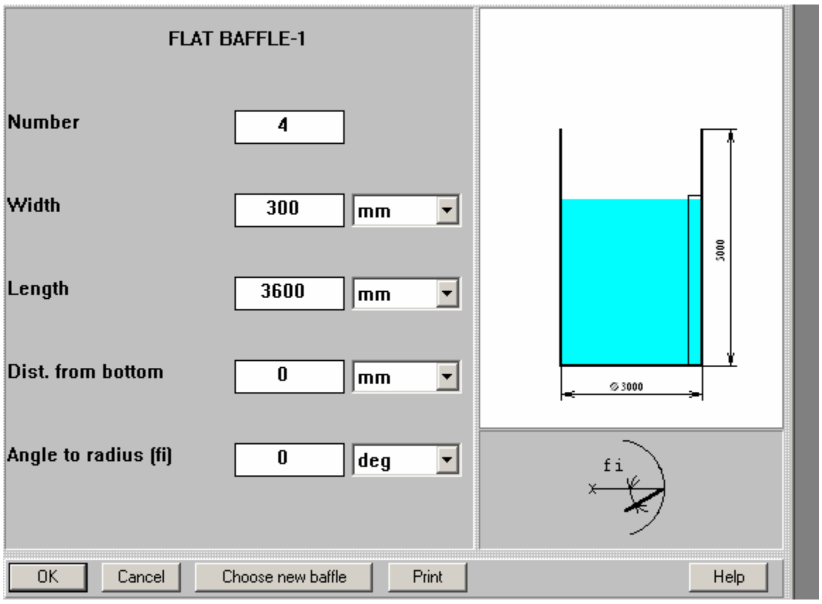


Figure 18.

It includes **flat baffles** used in steel tanks, and **tubular baffles** used mainly in glass-lined equipment. A steel baffled tank has typically a set of 3-4 baffles, the baffle width being 1/10 - 1/12 of the tank diameter. Glass-lined tanks are usually equipped with 1 or 2 tubular or Beavertail baffles fixed to the tank head.

When the scheme of the selected baffle appears (Figure 19), supply the requested baffle parameters.


FLAT BAFFLE-1

Number: 4

Width: 300 mm

Length: 3600 mm

Dist. from bottom: 0 mm

Angle to radius (fi): 0 deg

Figure 19.

If several baffles of different configurations are installed in the tank, an equivalent baffle should be entered, such that the radial projection of the baffle immersed area equals the average value for all baffles. The number of baffles entered should be the same as the actual number of baffles in the tank. The **Distance from wall** for the equivalent baffle must be equal to the average distance between the wall and the vertical axes of the baffles, and the **Distance from bottom** must equal the average baffle clearance.

NOTE: ***Inlet tubes, sensors and other fixed internal devices can be entered using Beavertail baffle of an appropriate cross-section.***

6.2.1. Flat baffles

Flat baffle -1 type corresponds to a flat baffle on the wall, Flat baffle-2 corresponds to a flat baffle at a distance from the wall.

Flat baffle-2 option can also be used for approximate calculations of other types of fixed internal devices, such as discharge tubes. In this case, a product of **Width** and **Length** of a baffle entered in the table should be equal to the radial cross-section of the fixed device. The value of **Distance from wall** must be selected so that the distance between the wall and the vertical axis of the fixed device equals the spacing between the wall and the vertical axis of the baffle.

NOTE: ***For radially installed baffles (both flat and tubular), the Angle to radius is zero.***

The distance between **Flat baffle-2** and the tank wall is usually about 1/3 - 1/4 of the baffle width.

6.2.2. Tubular baffles

These baffles have a tubular or flattened tubular cross-section. They are used mainly in glass-lined mixing tanks. The **Tube diameter** is usually about 1/10 of the tank radius.

6.2.3. De Dietrich Beavertail baffle

These baffles are mainly used in De Dietrich glass-lined equipment. One to three Beavertail baffles are usually installed in the tank; standard ratio of baffle and tank diameters is in the range 0.07-0.11.

6.3. Impellers

The procedure for selecting the impeller type and entering impeller data is similar to the one used for tanks and baffles. The impeller selection is shown in Figure 20.

The blue color in this graphic menu corresponds to glass-lined impellers characterized by their smooth surface and the streamlined configuration of the blades.

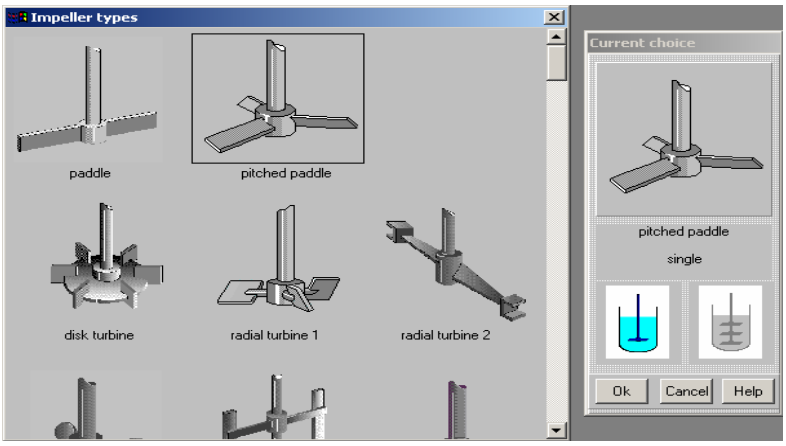


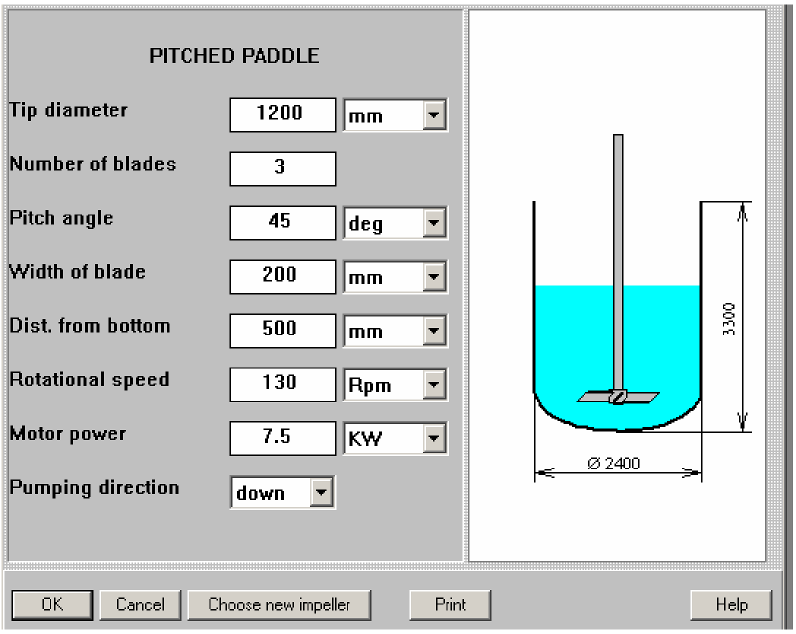
Figure 20.

You may choose impellers of most typical designs, both steel and glass-lined. After you have selected the impeller type, you can choose either a **single** (default) or a **multistage** system by clicking on the appropriate diagram in the **Current choice** window in the impeller selection screen. It is assumed that a multistage system consists of two or three identical impellers.

NOTE:
The impeller selection shown in the screen does not cover all impeller designs, which can be calculated by the program. If you want to perform calculations for an impeller, which is not shown in the IMPELLER TYPES screen, contact VisiMix technical support.

When the scheme of the selected impeller appears (Figure 21), supply the requested impeller parameters.

Width of blade is understood as actual width and not projected one.
Distance from bottom is impeller clearance, which is understood as the distance between the lowest point of the bottom, and the middle of the blade. The minimum allowable distance from bottom is about ¼ of the tank diameter for most impellers.
Motor power. Enter the rated power of the motor. This parameter is not used for calculations, and it is included in order to make sure that it is not exceeded by the mixing power.
The 30% reservation of power accepted in VisiMix is based on practical experience. It takes into account usual level of energy losses in electric drives with mechanical speed reducers (gyres). If the speed reduction is performed using electrical or electronic speed control devices, selection of the motor power has to be based on the rated torque moment of the low speed shaft that must be included in the technical characteristic of the drive. The recommended 30% reservation in this case must be related to the calculated **Torque** value.


PITCHED PADDLE

Tip diameter	1200	mm
Number of blades	3	
Pitch angle	45	deg
Width of blade	200	mm
Dist. from bottom	500	mm
Rotational speed	130	Rpm
Motor power	7.5	KW
Pumping direction	down	

Figure 21.

Pumping direction. The most common pumping direction for any impeller is **"down"**. For most single-stage impellers, VisiMix allows for selecting pumping direction, while for multistage impellers, **Pumping direction** cannot be selected and is always “**down”**. **Pumping direction** for vertical blades is of no importance.

NOTE:
When entering impeller data for a multistage system, take into account that VisiMix will disregard the upper impeller if it is placed too close to the surface or above the surface. This can also be seen in the visualization of the General flow pattern.

NOTE:
For multistage systems, the number of blades entered in the impeller input table is understood as the number of blades in a single impeller stage, and not as the total number of blades.

6.3.1. Anchor, frame

Compared to the Anchor impeller, the Frame impeller has an additional horizontal bar. This bar is used to prevent the winding of the impeller vertical arms. Its effect on the power and mixing process in turbulent regime is negligible. The **Tip diameter** of Anchor and Frame impellers is usually about 0.8 to 0.9 of the tank **Inside diameter**, and the **Width of blade** ("arm") is about 0.07 of the impeller **Tip diameter**.

6.3.2. Propeller

The propeller in the current version of VisiMix corresponds to a **marine screw** with a **Pitch = 1.0** (a blade angle of about 26 degrees). The **Tip diameter** is usually 1/4 to 1/3 of the tank diameter. The most common **Pumping direction** is **down.**

6.3.3. Disk turbine

The most typical design with vertical blades is a **Rushton turbine** with the following geometry: a pitch angle of 90 degrees; six blades; a disk diameter that is 0.75 of the **Tip diameter**; a blade width that is 0.2 of the **Tip diameter** and a blade length that is 0.25 of the **Tip diameter**. The **Tip diameter** of the Disk turbine impeller is usually less than 0.4 of the tank **Inside diameter**.

6.3.4. Pitch paddle

A common Pitch-paddle impeller, called also Pitch-blade turbine, PBT has 4-6 blades a Pitch angle of 45 degrees, however, pitch angles of 30 and 60 degrees are also used. For this impeller, the **Width of blade** is usually 0.15 – 0.25 of the **Tip diameter**, and the **Pumping direction** is down. The **Tip diameter** is usually 0.5 to 0.7 of the tank diameter. The program allows for choosing arbitrary impeller geometry. However, more than eight blades and a blade width greater than 0.3 of the **Tip diameter** are not recommended. **Pumping direction** for Pitch angle of 90 degrees is of no importance.

6.3.5. Paddle

For paddle impellers with vertical blades, the **Tip diameter** is usually 0.5 to 0.7 of the tank diameter. The number of blades is usually 2 to 6; the width of blades is 0.1 to 0.15 of the **Tip diameter**; the pumping direction is **down**. The blades of glass-lined impellers are usually made of tubes, and in such a way as to avoid sharp angles.

6.3.6. Lightnin A310

The blades of this impeller have a special hydrofoil configuration developed by the manufacturer in order to reduce energy losses. The pitch angle and geometric proportions of the impeller are fixed by the manufacturer, therefore the only variable parameters are the **Tip diameter** and the **Distance from bottom**.

6.3.7. Tooth-disk impellers

These impellers are mainly used for the preparation and homogenization of multi-component mixtures, such as paints, coatings, etc. They are driven by high speed drives with RPM of about 250-500; their tip velocity is usually 8-15 m/s or greater. Typically, the number of blades is 28 to 36.

6.3.8. De Dietrich

De Dietrich impeller

The blades of this glass-lined impeller are made of slightly flattened and curved tubes. The geometric proportions of the impeller are set by the manufacturer; therefore, the only variables are the **Tip diameter**, and the parameters describing the position of impeller in the tank, i.e. the **Distance from bottom**, and the **Distance between stages** for multistage systems. For the mixing of viscous media, the **Tip diameter** is usually 0.5 to 0.7 of the tank diameter.

De Dietrich GlasLock with Variable Flat Blades

De Dietrich glass-lined GlasLock impellers are used for various unit operations, including blending, mixing, homogenization, gas dispersion, suspension, heat transfer, crystallization, etc. They are designed with adjustable and removable blades, and can be used in both single and multistage applications.

De Dietrich GlasLock with Flat Blades

The typical pitch angles of GlasLock impellers with flat blades are:

30 degrees	recommended for suspension and crystallization
45 degrees	recommended for homogenization
60 degrees	general use for multipurpose reactors: blending, mixing, heat transfer
90 degrees	recommended for dispersion, gas absorption, gas-liquid reaction

The width of the blades is usually about 0.1 to 0.2 of the **Tip diameter**, the length of the blades is 0.1 to 0.25 of the **Tip diameter**. The standard number of blades is three.

De Dietrich GlasLock with Hydrofoil Blades

GlasLock impellers with hydrofoil blades ensure low power consumption and a high pumping capacity. They are used for suspension processes, heat transfer, and chemical reactions. The standard number of blades is three. The geometric proportions of the impeller are fixed by the manufacturer; therefore, the only variables are **Pitch angle**, **Tip diameter** and the parameters describing the position of the impeller in the tank, i.e. the **Distance from bottom**, and the **Distance between stages** for multistage systems.

De Dietrich GlasLock with Breaker Bar Blades

GlasLock impellers with Breaker Bar Blades are mainly used for viscous products. The standard pitch angles are 45 and 90 degrees, the standard number of blades is two. For the mixing of viscous media, the **Tip diameter** is usually 0.5 to 0.8 of the tank diameter.

6.3.9. Glass-lined paddle impellers

This option can be used for glass lined impellers of different design and dimensions, including those manufactured by Pfaudler, Tycoon, etc. It may also be used for polymer-lined impellers. Glass lining technology requires a streamlined configuration for all the elements of the impellers; therefore, the impeller blades are usually manufactured of flattened tubes.

6.3.10. Radial turbine

This option can be used for the calculations for a number of impellers produced by different manufacturers. For instance, for approximate simulation of a **INTERMIG** impeller, select **Radial turbine 2** and enter:

Pitch angle, fi = 26 degrees,
Width of blades, W = 0.1 Tip diameter;
Length of blades, L = 0.1 Tip diameter.

6.3.11. Scraper agitator.

Scraper agitators are used in tanks and reactors that require intensive heat transfer to a jacket. Their application is typical the cases when it is necessary to prevent adhesion of solid particles (for instance, in crystallizers, in reactors for precipitation processes, for suspension polymerization, etc.) or formation of a high viscosity film on the heat transfer surface of the tank.
Some kind of plastic, in the most cases -Teflon, is used as a material for the scrapers. The close contact of the scrapers to the tank wall is ensured due to flexibility of the plastic.

For input of scraper agitator you have to use **Supplement** option of the main menu.

6.4. Shafts.

Data in this part of the program are used for checking the suitability of the shaft based on the calculation of the critical frequency of shaft vibrations and maximum torsion stresses in dangerous cross-sections.
Calculations are based on the shaft sizes as preliminarily estimated and entered (see below). If the results of the calculations do not confirm the shaft reliability, the program issues appropriate messages. In this case, you should modify your input, e.g., increase the cross-section of the shaft section mentioned in the message, reduce the number of revolutions, etc.

The maximum torque of the selected impellers drive is used as initial data for Torsion stress calculation. For this reason, the mechanical calculations are always performed after the calculations of the hydrodynamics. The program automatically performs a preliminary check-up of the selected drive. If the drive does not correspond to the requirements described above, the program issues appropriate messages.

The program allows for two shafts schemes that differ by position of bearings with respect to the impellers:

- **Console shafts –** bearings are placed on the end of shaft opposite to the impellers. Usually the bearings are fixed on the tank cover (head) or on a special construction over the level of media. Impellers are fixed on the ‘console’ end of the shaft that is submerged in liquid media. However, the program can be applied for ‘bottom entering’ or ‘side entering’ shafts.
- **Beam shafts –** bearings are placed on both ends of the shaft, and impellers are fixed between the bearings. Such shafts are described also as ‘shafts with end bearing’ or ‘shafts with submerged bearing’.

All shaft sections are assumed to be made of the same metal with identical mechanical properties. Calculations can also be performed for glass-lined shafts and shafts with other coatings. However, applicability of the VisiMix suitability criteria is not guaranteed for these cases.

Calculations are performed for shafts with two to five impellers fixed on different distances from the bearings.

6.4.1. Shaft design

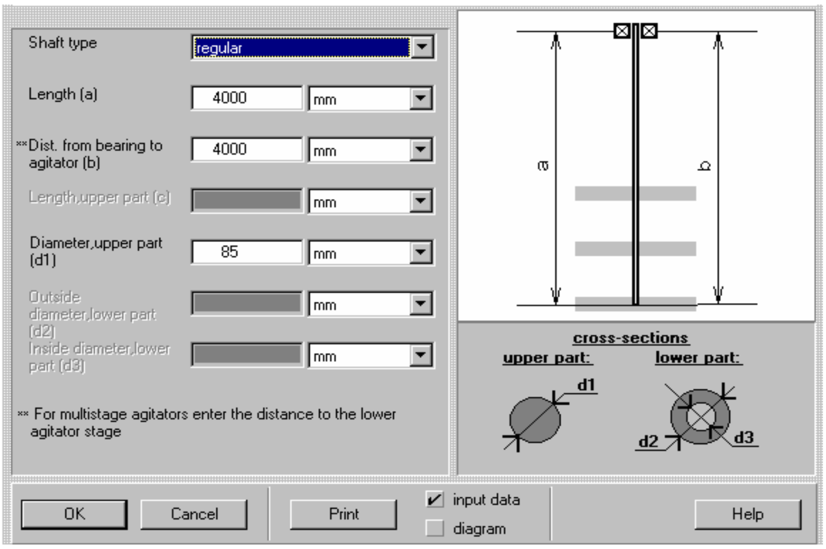
Four types of shafts are considered:

- A solid stiff console shaft with a constant diameter (**console regular**);
- A stiff console shaft consisting of two parts of different diameters (**console combined**);
- A solid stiff beam shaft with a constant diameter (**beam regular**);

- A stiff beam shaft consisting of two parts of different diameters (**beam combined**);

A built-up shaft with stiff couplings is regarded as a single item.

The term “stiff shaft” means that the rotational frequency of the shaft is less than the shaft’s critical (resonance) frequency of vibrations.



Shaft type: regular
Length (a): 4000 mm
**Dist. from bearing to agitator (b): 4000 mm
Length,upper part (c): mm
Diameter,upper part (d1): 85 mm
Outside diameter,lower part (d2): mm
Inside diameter,lower part (d3): mm

** For multistage agitators enter the distance to the lower agitator stage

☑ input data
☐ diagram

Figure 22.

- **Length (a).** This parameter is related to the ‘loaded’ part of the shaft. For console shafts you enter length of the console, i.e. distance between the cross-section of the lower bearing and the end of the shaft. For beam shafts distance between bearings is entered.
  A built-up shaft with stiff couplings is regarded as a single item.

- **Distance between bearings (b)** is entered for console shafts only. Influence of this parameters for the regular shafts is not significant. If the distance is unknown, enter 0. In this case the program performs calculations for b = a/4, that corresponds in the most cases to the maximum reservation.

- **Upper part (length, diameter).** For a combined shaft, the upper section is the section between the cross-section of the bearing and the cross-section corresponding to the change of the shaft diameter. For a regular shaft, the whole shaft is considered as the upper section.

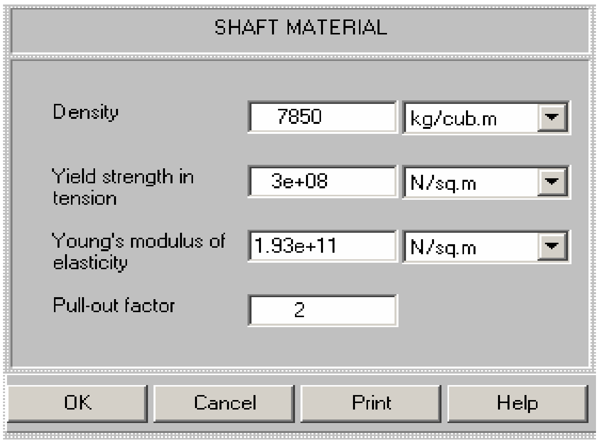
- **Diameter between bearings (d0)** is required for combined console shafts only. If this diameter is unknown, you are asked to enter 0 for approximate calculation. In this case the d0 is assumed to be equal to diameter of the upper shaft section (d0 = d).

- **Lower part (outside and inside diameters).** For a shaft with a solid lower section, enter “0” as an inside diameter.

6.4.2. Shaft material.

Enter the properties of the shaft material: **Density, Yield strength, Young's modulus of elasticity** (Figure 23).

Some typical values of Yield strength and Young's modulus of elasticity for a number of commonly used materials is presented in the Table 3 (given according to Mechanics of Materials, SI Metric Edition, F. P. Beer, E. R. Johnston, Jr., McGraw-Hill, 1985, and Mixing in the Process Industries, Second Edition, N. Harnby, M. F. Edwards, A. W. Nienow, Butterworth - Heinemann, 1992).



SHAFT MATERIAL

Density: 7850 kg/cub.m

Yield strength in tension: 3e+08 N/sq.m

Young's modulus of elasticity: 1.93e+11 N/sq.m

Pull-out factor: 2

Figure 23.

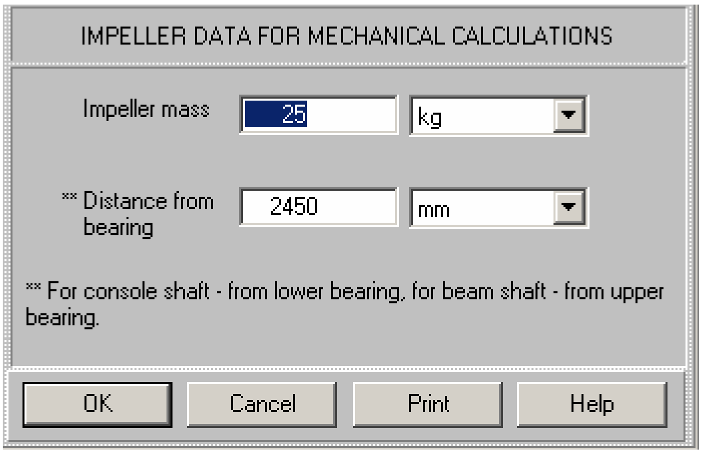
The actual values of these properties depend on shaft shape and dimensions, heat treatment and composition of the material. Density for different steels lies in the range 7700 - 8000 kg/m3 For Titanium, the density is 4500 kg/m3.

Table 2. Yield strength and Young's modulus of elasticity

Material	**Properties**			
	Yield strength		**Young modulus of elasticity**	
	N/sq. m	psi	N/sq. m	psi
Structural steel	2.6 E+8	3.77 E+4	2 E+11	2.9 E+7
High strength-low alloyed steel	3.5 E+8	5.08 E+4	2 E+11	2.9 E+7
Quenched and tempered alloyed steel	7 E+8	1.02 E+5	2 E+11	2.9 E+7
Stainless cold-rolled steel	5÷11 E+8	7.25÷16 E+4	1.93 E+11	2.8 E+7
Stainless annealed steel	2.05÷2.75 E+8	2.97÷3.99 E+4	1.93 E+11	2.8 E+7
Titanium	5.15 E+8	7.47 E+4	1.03 E+11	1.49 E+7

6.4.3. Impellers data for mechanical calculations.

- **Mass of impellers**. The mass of each impeller has to be entered accordingly to its position on the shaft. The numbers of impellers in this table corresponds to their numbers in the Mixing device input table.



IMPELLER DATA FOR MECHANICAL CALCULATIONS

Impeller mass: 25 kg

** Distance from bearing: 2450 mm

** For console shaft - from lower bearing, for beam shaft - from upper bearing.

Figure 24.

- **Distance from bearing to impeller** . For console shafts enter the distance from the central cross-section of the impeller placed close to the lower end of the shaft to the cross-section of the lower bearing. For beam shafts the distance from this impeller to the upper bearing is entered. Positions of other Impellers are defined by the program accordingly to the previous inputs.

6.5. Properties & Regime

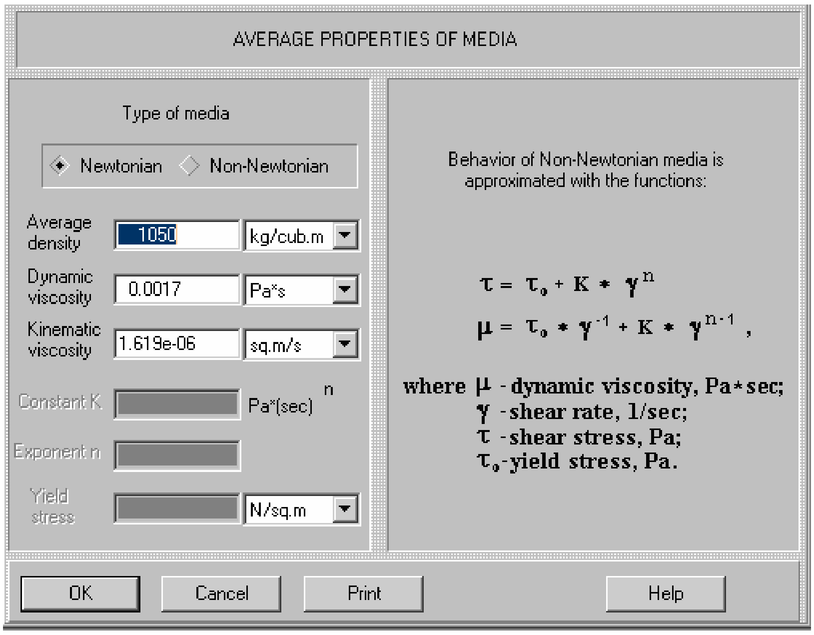
6.5.1. Average properties of media

Select media type - Newtonian or Non-Newtonian (Figure 24) - and provide the data based on measurements or reference data.

For the Newtonian option, enter the available viscosity value (either dynamic or kinematic), and the program will calculate the other viscosity value.

For the non-Newtonian option, calculations are based on a universal rheological model shown in this input table. If you describe the behavior of your media with a different model, we recommend approximating the rheological function with the equations adduced here.

NOTE:
Contact VisiMix technical department for more information about this function.



AVERAGE PROPERTIES OF MEDIA

Type of media

● Newtonian ○ Non-Newtonian

Average density: 1050 kg/cub.m

Dynamic viscosity: 0.0017 Pa*s

Kinematic viscosity: 1.619e-06 sq.m/s

Constant K: Pa*(sec) ^{n}

Exponent n:

Yield stress: N/sq.m

Behavior of Non-Newtonian media is approximated with the functions:

$$\tau = \tau_o + K * \gamma^n$$

$$\mu = \tau_o * \gamma^{-1} + K * \gamma^{n-1},$$

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

Figure 25.

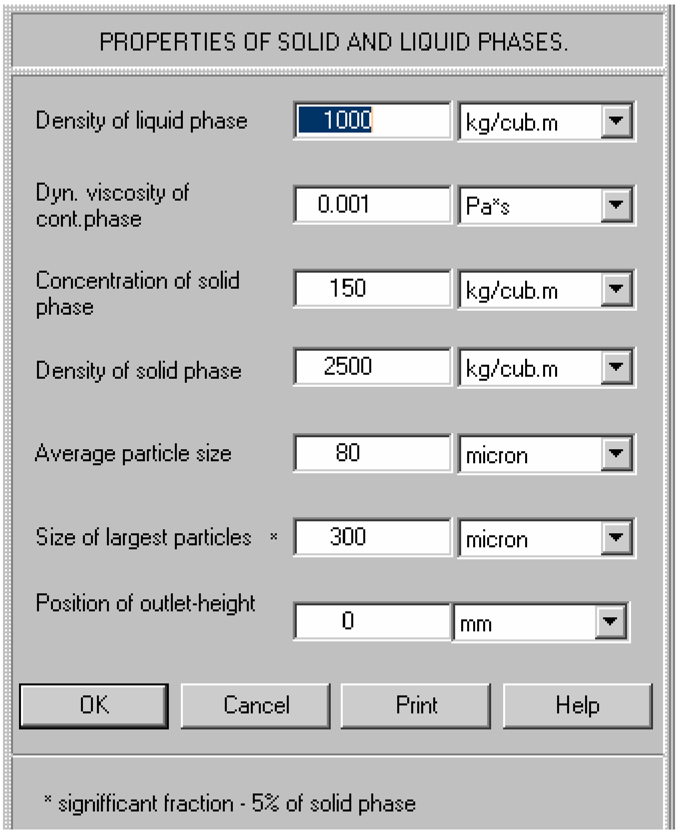
Data entered in this table are used for calculation of **Hydrodynamics**, **Turbulence** and **Single-phase liquid mixing**.

NOTE:
If you do not know the exact values, enter approximate ones. For turbulent regimes, small errors in estimation of viscosity are usually not important. For density, accuracy is more important because mixing power is proportional to the density value.

6.5.2. Properties of solid and liquid phases

You will be asked to fill in this table (Figure 26) for modeling **Liquid-solid mixing**.

Concentration of solid phase. For batch processes, the concentration of the solid phase is understood as the average concentration in the tank; for continuous flow processes it is understood as the concentration in the feed flow. This parameter is also used for calculation of dissolution processes, in which it is understood as the initial concentration of the solid phase.



PROPERTIES OF SOLID AND LIQUID PHASES.

Density of liquid phase 1000 kg/cub.m

Dyn. viscosity of cont.phase 0.001 Pa*s

Concentration of solid phase 150 kg/cub.m

Density of solid phase 2500 kg/cub.m

Average particle size 80 micron

Size of largest particles * 300 micron

Position of outlet-height 0 mm

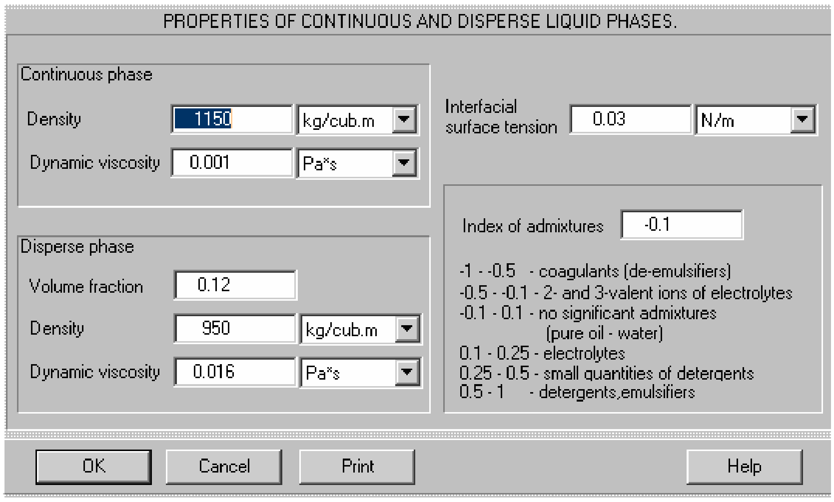
* signifficant fraction - 5% of solid phase

Figure 26.

The **Position of outlet** is significant for continuous flow regime only, i.e. for a continuous suspension inlet and outlet with a constant flow rate. For a batch mixing tank, enter any positive number. This data is also needed for calculations of solid-liquid mass transfer (dissolution).

6.5.3. Properties of continuous and disperse liquid phases

You will be asked to fill in this table (Figure 27) when first addressing a parameter from the **Liquid-liquid mixing** submenu.



PROPERTIES OF CONTINUOUS AND DISPERSE LIQUID PHASES.

Continuous phase

Density 1150 kg/cub.m

Dynamic viscosity 0.001 Pa*s

Interfacial surface tension 0.03 N/m

Disperse phase

Volume fraction 0.12

Density 950 kg/cub.m

Dynamic viscosity 0.016 Pa*s

Index of admixtures -0.1

-1 - -0.5 - coagulants (de-emulsifiers)
-0.5 - -0.1 - 2- and 3-valent ions of electrolytes
-0.1 - 0.1 - no significant admixtures (pure oil - water)
0.1 - 0.25 - electrolytes
0.25 - 0.5 - small quantities of detergents
0.5 - 1 - detergents,emulsifiers

Figure 27.

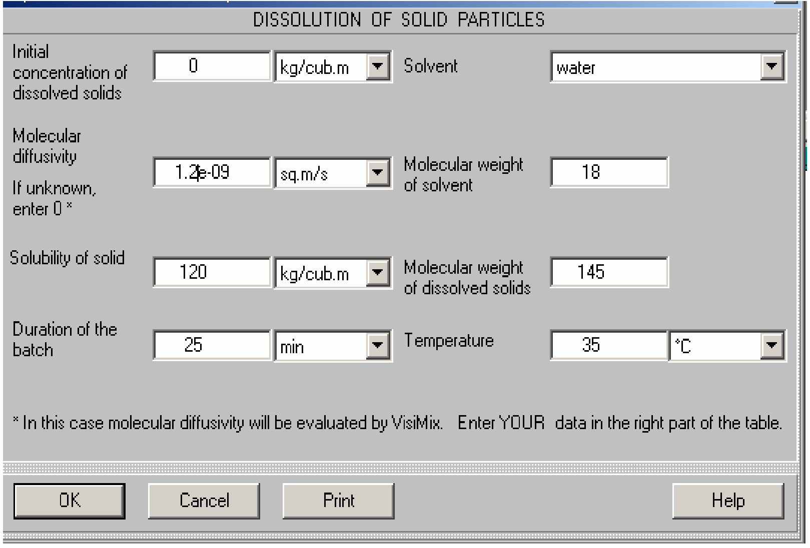
Besides the obvious physical properties of a two-phase system, the program takes into account the electrostatic restricting pressure on the oil-water surface, which reduces the probability of the droplet coalescence.

Interfacial surface tension. If the exact value is unknown, enter an approximate one. For the majority of oil-water couples, interfacial surface tension is about 0.02 - 0.03 N/m; for emulsions stabilized with emulsifiers, the surface tension drops to 0.01 - 0.015 N/m.

Index of admixtures. Kinetics of coalescence of droplets and drop size distribution depend on the repulsive pressure of the double layers formed on the interface. The estimation of this pressure is based on the **Index of admixtures.** Evaluate and enter the **Index of admixtures** with respect to the composition of the emulsion.

6.5.4. Dissolution of solid particles (Liquid-solid mass transfer)

You will be asked to fill in this table (Figure 28) for simulation of a dissolution process.



DISSOLUTION OF SOLID PARTICLES

Initial concentration of dissolved solids: 0 kg/cub.m
Solvent: water
Molecular diffusivity If unknown, enter 0 *: 1.2e-09 sq.m/s
Molecular weight of solvent: 18
Solubility of solid: 120 kg/cub.m
Molecular weight of dissolved solids: 145
Duration of the batch: 25 min
Temperature: 35 °C

* In this case molecular diffusivity will be evaluated by VisiMix. Enter YOUR data in the right part of the table.

Figure 28.

The table contains a list of specific initial data for mass transfer calculations, including the solubility of the solid (concentration of saturation) and diffusivity of the dissolved solids in the liquid solvent. If the molecular diffusivity of the dissolved solid in the solvent is unknown, VisiMix will calculate it. In this case, enter **‘0’**, and the boxes in the right part of the table will become active. Enter your data, disregarding some irrelevant figures that will appear in these boxes. VisiMix includes equations for the approximate calculation of diffusivity of different substances in three kinds of solvents - water, organic alcohols and other organic liquids. The **Solubility of solid phase** cannot be calculated and must be entered according to reference or practical data for the specific solid-solvent couple.

NOTE:
The value for initial concentration of the solid phase in suspension, which is necessary for all calculations of dissolution processes, is absent from this table, since it is assumed equal to Concentration of solid phase entered in PROPERTIES OF SOLID AND LIQUID PHASES input table.

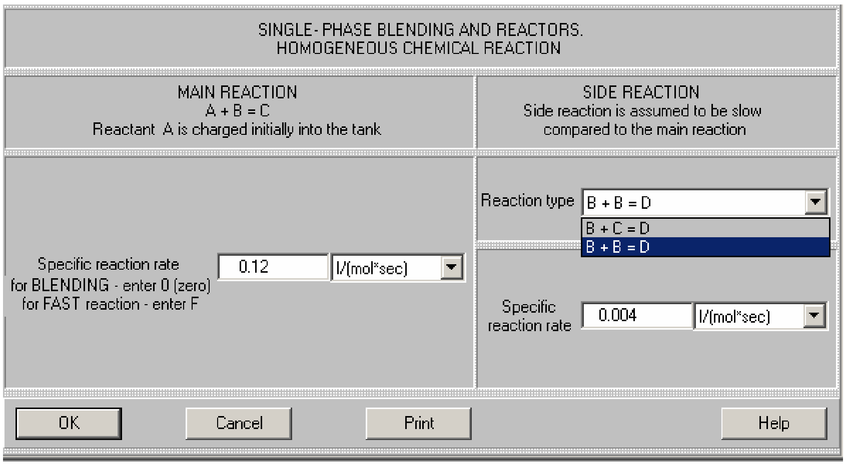
Calculation of the dissolution time is only performed if the sum of the **Concentration of solid phase** entered in PROPERTIES OF SOLID AND LIQUID PHASES input table and the **Initial concentration of dissolved solids** entered in this table, is lower than the solubility of the solid phase. If the **Concentration of solid phase**, or **Initial concentration of dissolved solids** is too high, VisiMix issues a message indicating that the complete dissolution is impossible.

The **Liquid-solid mass transfer** section in the current version of VisiMix performs simulation of dissolution only. However, calculated values of mass transfer coefficient may also be used for the analysis and calculation of the solid-liquid extraction (leaching) and crystallization.

6.5.5. Single-phase blending and chemical reaction

Chemical reaction data.

You will be asked to fill in the table SINGLE-PHASE BLENDING AND REACTORS. HOMOGENEOUS CHEMICAL REACTION (Figure 29) for modeling **Batch reaction/blending, Semibatch** and **Continuous flow reaction**.



SINGLE- PHASE BLENDING AND REACTORS.
HOMOGENEOUS CHEMICAL REACTION

MAIN REACTION
A + B = C
Reactant A is charged initially into the tank

Specific reaction rate
for BLENDING - enter 0 (zero)
for FAST reaction - enter F
0.12 l/(mol*sec)

SIDE REACTION
Side reaction is assumed to be slow
compared to the main reaction

Reaction type: B + B = D

Specific reaction rate: 0.004 l/(mol*sec)

Figure 29.

The data on the reaction kinetics is required for the simulation of distribution of local concentrations of reactants in a real (“non-perfect”) reactor as a function of the reactor and impeller design. This data also allows for evaluating the selectivity of the reaction accompanied with a parallel side reaction.

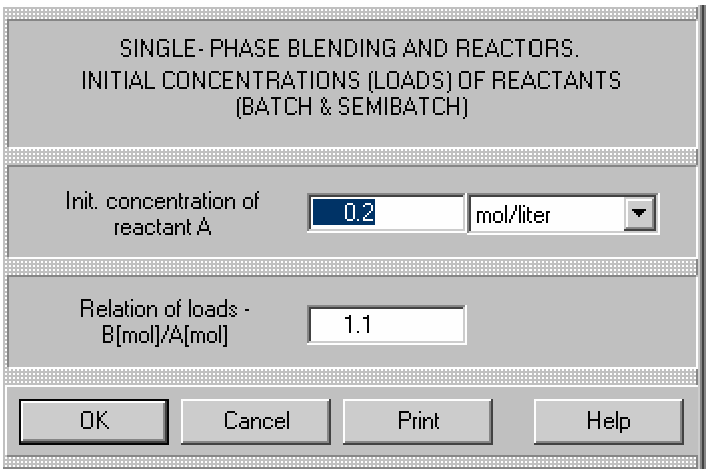
Enter the following data:

- data for the main reaction (A+B→C);

- the type of the side reaction, by selecting B+B→D or B+C→D option
- specific reaction rate for the side reaction, which must not be higher than 0.2 of the specific rate value for the main reaction.

For reactions without by-products, enter “**0**” as specific reaction rate for the side reaction.

If the specific reaction rate for the main reaction is not known, enter "**F**" ("fast chemical reaction"). In this case, the program will provide the maximum limit of non-uniformity in the tank. If there is no chemical reaction, enter **"0"**, and the program will simulate distribution of tracer or other substances that are injected as a solution in the same solvent (blending).


SINGLE- PHASE BLENDING AND REACTORS.
INITIAL CONCENTRATIONS (LOADS) OF REACTANTS
(BATCH & SEMIBATCH)

Init. concentration of reactant A: 0.2 mol/liter

Relation of loads - B[mol]/A[mol]: 1.1

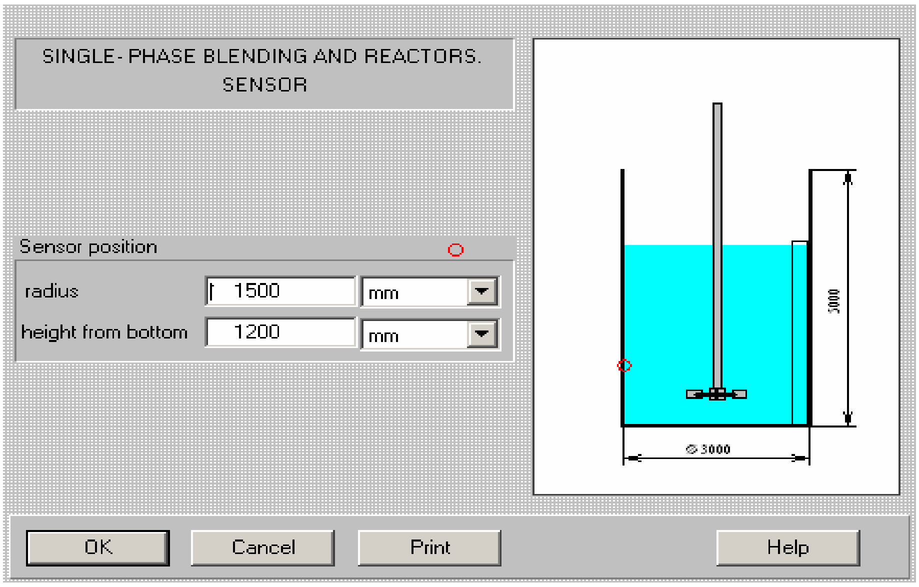
Figure 30.

Concentrations of reactants (Batch & Semi-batch)

Initial concentrations of reactants (Figure 30) and concentrations of products in the VisiMix sections related to chemical reactions are expressed in molar units. It is possible to enter concentrations in g-mol. per liter or in kg-mol. per cub.meter of the reaction media .

Sensor position.

You will be asked to fill in this table (Figure 31) for modeling **Continuous flow dynamics, Batch reaction/blending, Semibatch** and **Continuous flow reaction**.



SINGLE- PHASE BLENDING AND REACTORS.
SENSOR

Sensor position

radius 1500 mm

height from bottom 1200 mm

Figure 31.

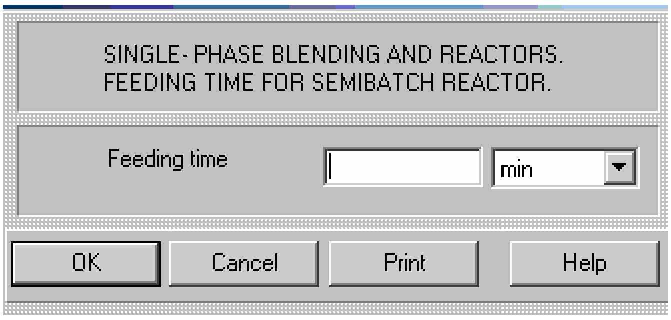
You may also follow the change of concentrations in any chosen point of the volume by entering the corresponding coordinates in the **Sensor position** input box. If you are not interested in any specific point, enter any positive number.

Inlet position.

For simulation of **Batch** and **Semibatch** reactors it is necessary to define point of inlet of reactant B. It is supposed that the reactant A is uniformly distributed in the reactor before start of the reactant B adding.

Semibatch reactor (feeding time)

It is assumed that reactant B is loaded into a semibatch reactor with a constant flow rate during a certain period. Enter the duration of this period as **Feeding time** in the input table in Figure 32.



SINGLE- PHASE BLENDING AND REACTORS.
FEEDING TIME FOR SEMIBATCH REACTOR.

Feeding time min

Figure 32.

Specific parameters for continuous flow reactors.

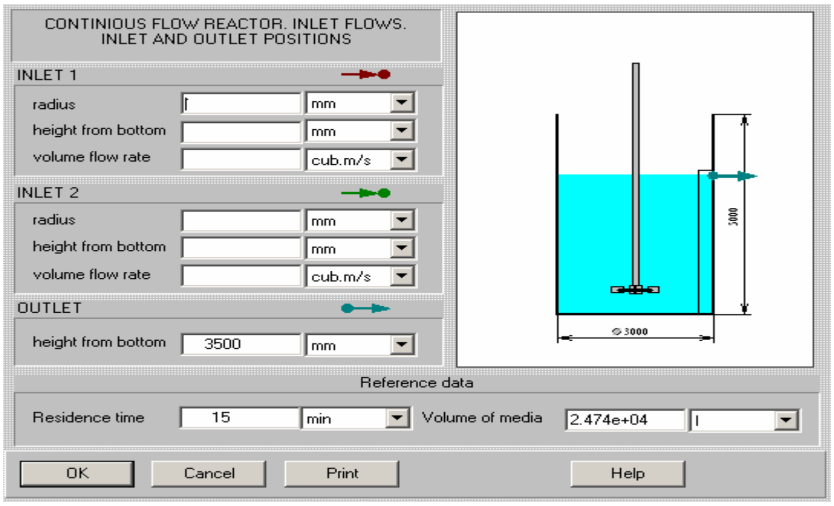
Inlet and outlet positions.

It is supposed that the reactor is equipped with two **Inlet** and single **Outlet** pipes.

For **Inlet 1** and **Inlet 2** specify radius, height from bottom, and **Volume flow rate**. If the reactants are entered using single inlet pipe, you may enter coordinates of this **Inlet** point as **Inlet 1**. For **Inlet 2** in such cases any positive numbers for coordinates and **'0'** for **Volume flow rate** may be entered.

Position of **Outlet** specify height from bottom. For bottoms other than flat, this distance is measured from the lowest point of the bottom. For outlet pipes located at the media level, you may enter any value which is greater than the media level, for example, the tank height, and VisiMix will default to the **Level of media** which you entered in the **TANK** input table.
Media volume is presented in this screen for reference. It corresponds to the User's input in the **TANK** input table.

The **Residence time** - mean residence time of the media in the reactor - is calculated as the ratio **(Volume flow rate, inlet 1 + Volume flow rate, inlet 2) / Media volume.**


CONTINIOUS FLOW REACTOR. INLET FLOWS.
INLET AND OUTLET POSITIONS

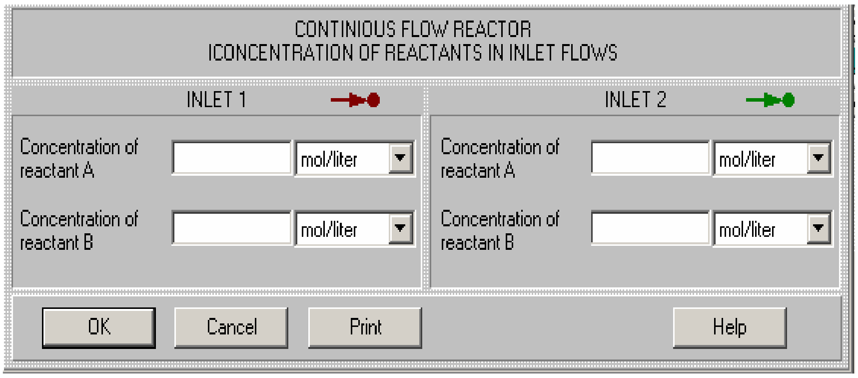
INLET 1
radius: mm
height from bottom: mm
volume flow rate: cub.m/s

INLET 2
radius: mm
height from bottom: mm
volume flow rate: cub.m/s

OUTLET
height from bottom: 3500 mm

Reference data
Residence time: 15 min
Volume of media: 2.474e+04 l

Figure 33.


CONTINIOUS FLOW REACTOR
ICONCENTRATION OF REACTANTS IN INLET FLOWS

INLET 1
Concentration of reactant A: mol/liter
Concentration of reactant B: mol/liter

INLET 2
Concentration of reactant A: mol/liter
Concentration of reactant B: mol/liter

Figure 34.

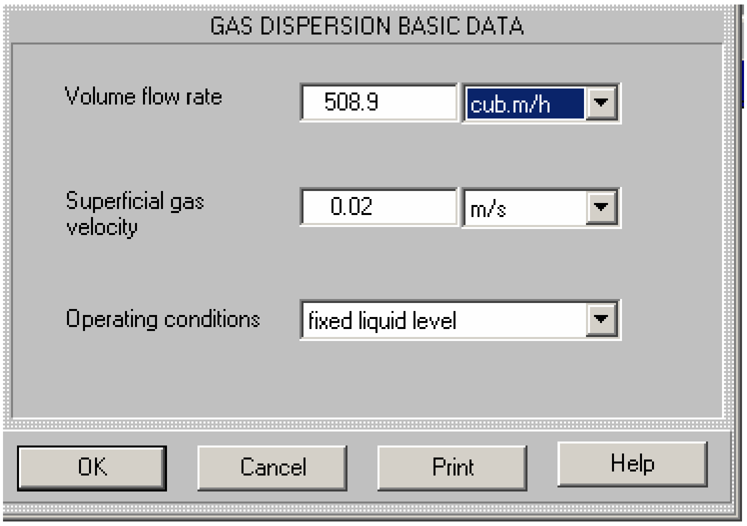
This input table specifies concentrations of reactants A and B foin the **Concentration of reactants in inlet flows.**

flows that are injected through the **Inlet 1** and **Inlet 2.** The most usual conditions correspond to separate inlet of the reactants: concentration of one of the reactants in each inlet is ‘0’.

6.5.6. Gas dispersion and mass transfer.

Gas dispersion basic data

Simulation of gas dispersion and mass transfer in gas-liquid systems requires additional initial data. The minimum set of data required for any Gas-Liquid calculations is shown in Figure 35.



GAS DISPERSION BASIC DATA

Volume flow rate: 508.9 cub.m/h

Superficial gas velocity: 0.02 m/s

Operating conditions: fixed liquid level

Figure 35.

Enter either the **Volume flow rate**, or the **Superficial gas velocity**, and the second parameter will be calculated by the program and entered automatically.

- **Volume flow rate**. This is the volume flow rate of gas introduced through a sparger installed under the lower (bottom) agitator. You must define this value with respect to working pressure and temperature in the tank. If a significant part of gas is absorbed in the tank, the final flow rate of the gas must be entered.
- **Superficial gas velocity** is the volume flow rate of gas per unit of the tank cross-section. You must define this value with respect to working pressure and temperature in the tank. If you enter the value for the **Volume flow rate** in this input table, the **Superficial gas velocity** is calculated as the **Volume flow rate** divided by the cross-section of the tank. Calculations are performed for values of the **Superficial gas velocity** in the range of 0 to 0.05 m/s.

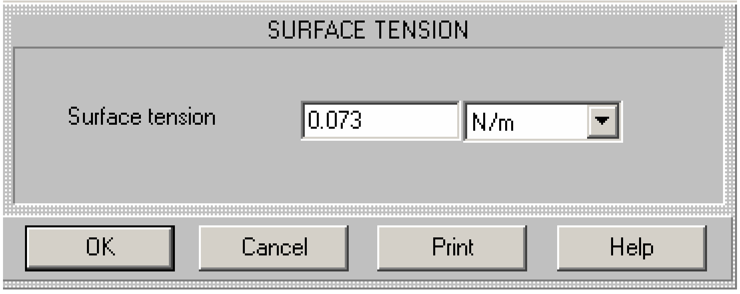
- **Operating conditions**. You can choose one of the two options: **Fixed liquid level**, or **Fixed liquid volume.** These options define process conditions typical for gas-liquid operations.

- **Fixed liquid level.** This option is selected for **Continuous flow** reactors, in which the level of media is usually fixed by position of the outlet pipe. In this case, the level of the media remains constant while gas is injected into the tank, but volume of liquide in the tank is reduced accordingly to the **Gas hold-up .**

- **Fixed liquid volume.** This option is selected mainly for **batch** processes, in which the media level in the tank after gas injection is higher than the initial level, in proportion to the **Gas hold-up** value. In this case, the quantity of the media in the tank remains constant after gas is injected into the tank.

Surface tension

Surface tension on the gas-liquid surface is a physical parameter of the system, which depends mainly on chemical composition of the phases,


SURFACE TENSION

Surface tension 0.073 N/m

Figure 36.

and on the working temperature. This parameter is necessary for modeling bubble break-up in the turbulent flow. Its value must be entered from reference data, or from the results of laboratory measurements. For the water-air interface at 20°C, it is 0.072 N/m.
The **Surface tension** values for some liquids are given in the table below and in the **Help** section. For direct access to these data the **Help** button in the **Surface tension** input screen is used.

Table 3. Surface tension of liquids on the air interface, N/m

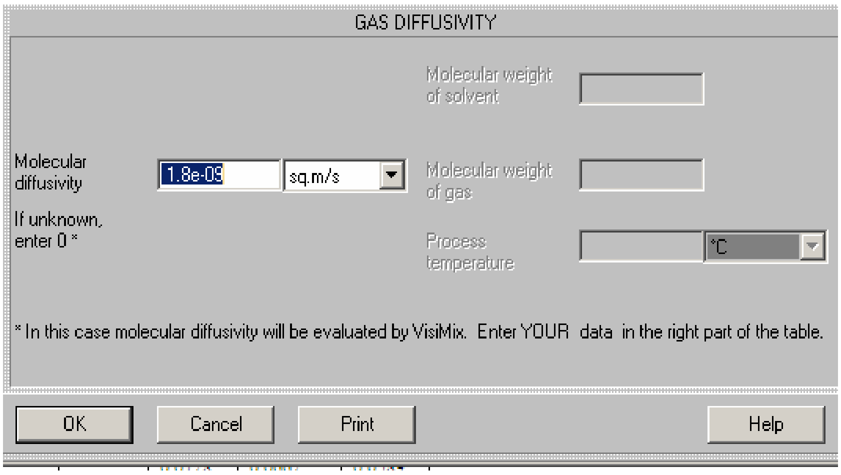
Substances	**Temperature, °C**			
	-20	20	60	100
Ammonium, water solution 25%	-	0.0629	0.0563	0.049
Aniline		0.0429	0.0383	0.0337
Bensol		0.029	0.0237	0.0188
Butyl alcohol	0.028	0.0246	0.0212	0.0178
Hexane	0.0226	0.0184	0.0142	0.010
Glycerol, water solution, 50%		0.0696	0.063	0.0557
Diethyl ether	0.022	0.017	0.0124	0.008
Sodium hydroxide (caustic), 50%		0.130	0.129	0.128
30%		0.097	0.096	0.0944
10%		0.0773	0.075	0.0707
Sulfuric acid, 98%		0.0551	0.0537	0.0525
75%	0.0741	0.0731	0.0721	0.0711
60%	0.0773	0.0761	0.0745	0.0727
Water		0.0728	0.0662	0.0589
Sodium chloride, 20%		0.080	0.0732	0.0659

Gas diffusivity

The value for the **Molecular diffusivity** of the gaseous component in the liquid is necessary for mass transfer calculations. It is entered in the table shown in Figure 37.

Molecular diffusivity values for some gases in water at 20°C are given in the table below (after B. I. Brounstein and A. S. Zelezniak, Physical Foundations of Liquid Extraction, Khimia Publishing House, Moscow-Leningrad, 1966).

For direct access to these data the **Help** button in the input screen is used. If the molecular diffusivity is unknown, VisiMix will calculate it. In this case, enter ‘**0’**, and the boxes in the right part of the table will become active. Enter your data, disregarding some irrelevant figures that will appear in these boxes.



Molecular diffusivity 1.8e-09 sq.m/s

If unknown, enter 0 *

* In this case molecular diffusivity will be evaluated by VisiMix. Enter YOUR data in the right part of the table.

Figure 37.

Table 4. Diffusivity of different gases in water at 20^0 C.

Substance	**Diffusivity, sq. m/s**
Carbon dioxide – CO2	1.50e-9
Chlorine	1.40e-9
Hydrogen chloride	3.14e-9
Hydrogen	3.59e-9
Ammonium	1.08 e-9
Acetylene	1.76 e-9
Oxygen	1.80 e-9

Gas solubility

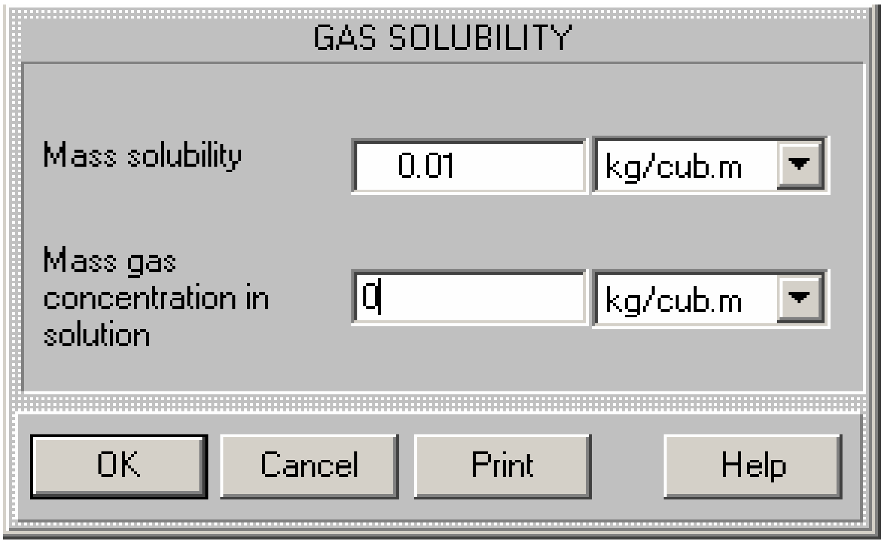
The **Mass solubility** of the gaseous component in liquid cannot be calculated and must be entered from reference or practical data for each individual gas-liquid couple (Figure 38).

It is assumed that the solubility value entered in this table corresponds to the pressure and chemical composition of the gaseous mixture exiting the liquid at the temperature of the liquid.

The program calculates the instant value of the mass transfer rate corresponding to this value of the solubility and to the **Mass gas concentration in solution**, which is entered in the same input table.

Solubility values for some gases in water at partial pressure of 1.013e5 Pa (1 bar) are given in the table below, after *Short Handbook on Chemistry*, Ed. D. Kurilenko, Publ. House “Naukova Dumka”, Kiew, Ukraina, 1974. For direct access to these data the **Help** button in the input screen is used.

Solubility values for some gases in water at partial pressure of 1.013e5 Pa (1 bar) are given in the table below, after *Short Handbook on Chemistry*, Ed. D. Kurilenko, Publ. House “Naukova Dumka”, Kiew, Ukraina, 1974. For direct access to these data the **Help** button in the input screen is used.



GAS SOLUBILITY

Mass solubility: 0.01 kg/cub.m

Mass gas concentration in solution: 0 kg/cub.m

Figure 38.

Table 5. Solubility of some gases in water

Gas	**Solubility, kg per cub. m**			
	Temperature, °C			
	0	20	60	100
Ar	0.10	0.060	0.040	
CH_4	0.040	0.024	0.014	
C_3H_8		0.074		
C_4H_{10}		0.085		
C_2H_2	2.01	1.22		
C_2H_4	0.28	0.152		
Cl_2	14.4	7.1	3.2	0
$Cl\ O_2$	27.6	87.0		
C O	0.044	0.028	0.015	0
$C\ O_2$	3.37	1.72	0.705	
H_2	0.0019	0.0016	0.00115	0
H_2S	6.63	4.41		
NH_3	467	345	156	
N O	0.10	0.063	0.040	0.035
O_2	0.070	0.0442	0.028	0.024
O_3	0.037	0.020	0	
SO_2		94	32	

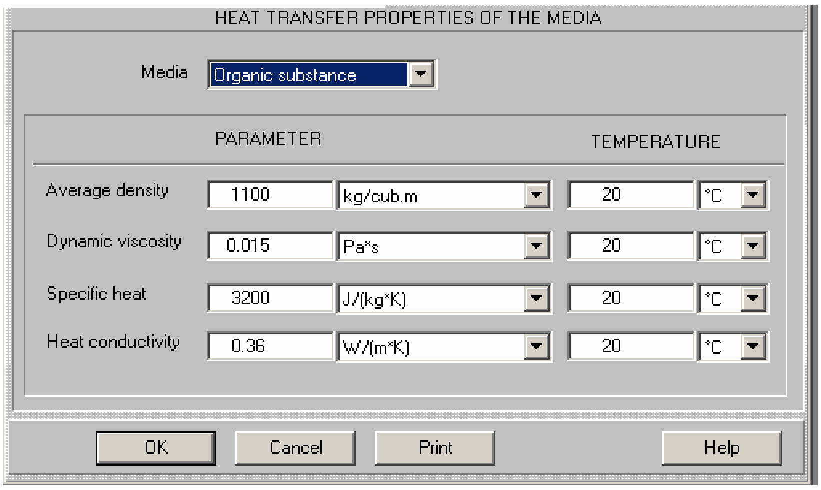
6.5.7. Heat transfer

Heat transfer properties of the media

Heat transfer calculations and modeling of heating/cooling dynamics is performed with respect to the change in the physical properties of the media as a function of the temperature. Calculations are based on approximate empirical correlations and on the values of properties available for any single temperature value. These correlations differ for water solutions and organic substances. Specify the **Media (Water solution** or **Organic substance)** and enter the values of the media properties and the corresponding temperatures (Figure 39). See APPENDIX 3 for reference data on the properties.

Chemical reaction data and regime

The program performs simulation of temperature regime for chemical reaction with heat release or consumption based on the kinetic and thermodynamic data entered in this table (Figure 40).

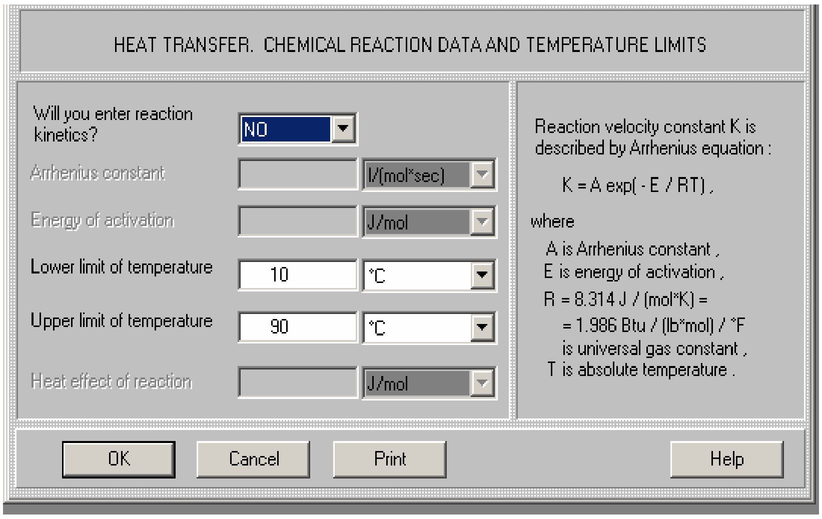


HEAT TRANSFER PROPERTIES OF THE MEDIA

Media: Organic substance

PARAMETER			TEMPERATURE	
Average density	1100	kg/cub.m	20	°C
Dynamic viscosity	0.015	Pa*s	20	°C
Specific heat	3200	J/(kg*K)	20	°C
Heat conductivity	0.36	W/(m*K)	20	°C

Figure 39.



HEAT TRANSFER. CHEMICAL REACTION DATA AND TEMPERATURE LIMITS

Will you enter reaction kinetics?	NO	
Arrhenius constant		l/(mol*sec)
Energy of activation		J/mol
Lower limit of temperature	10	°C
Upper limit of temperature	90	°C
Heat effect of reaction		J/mol

Reaction velocity constant K is described by Arrhenius equation :

K = A exp(- E / RT) ,

where

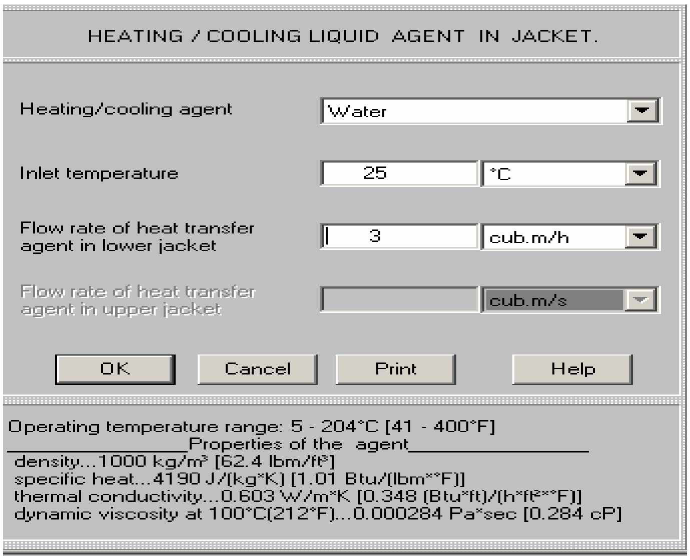
A is Arrhenius constant ,
E is energy of activation ,
R = 8.314 J / (mol*K) =
= 1.986 Btu / (lb*mol) / °F
is universal gas constant ,
T is absolute temperature .

Figure 40.

Choose **YES** if you want to enter the data on chemical reaction, and the corresponding boxes in the table will be activated. Choose **NO** if the exact kinetic data or the **Heat effect of reaction** is not known. In this case you will be asked to enter the available approximate data on the **Average rate of heat release (consumption)** or **Heat release (consumption) for a batch** in the input tables that follow. In all cases, specify the range of the process temperatures by entering the **Lower** and **Upper limit of temperature** for the media.

Liquid Heating/cooling agent. Convection in jacket

The program performs heat transfer calculations and modeling for tanks with all commonly used heating/cooling agents. Choose the heating/cooling agent (Figure 41) and enter the **Inlet temperature** and **Inlet flow rate** for the lower jacket section. Enter the **Inlet flow rate** for the upper jacket section if you have selected a 2-section jacket with the sections connected **in parallel** for the current project.
The practical range of operating temperatures and properties of the selected agent are shown in the lower part of the table. If the range of the process temperatures you have previously entered in HEAT TRANSFER. CHEMICAL REACTION DATA AND TEMPERATURE LIMITS input table falls partly or entirely outside the range of operating temperatures for the selected liquid agent, VisiMix issues a message indicating that the selected agent does not correspond to the indicated range of the process temperatures. In this case, select another heating agent or modify the process temperature range.



Heating/cooling agent: Water

Inlet temperature: 25 °C

Flow rate of heat transfer agent in lower jacket: 3 cub.m/h

Flow rate of heat transfer agent in upper jacket: cub.m/s

```
Operating temperature range: 5 - 204°C [41 - 400°F]
____________________Properties of the  agent____________________
 density...1000 kg/m³ [62.4 lbm/ft³]
 specific heat...4190 J/(kg*K) [1.01 Btu/(lbm*°F)]
 thermal conductivity...0.603 W/m*K [0.348 (Btu*ft)/(h*ft²*°F)]
 dynamic viscosity at 100°C(212°F)...0.000284 Pa*sec [0.284 cP]
```

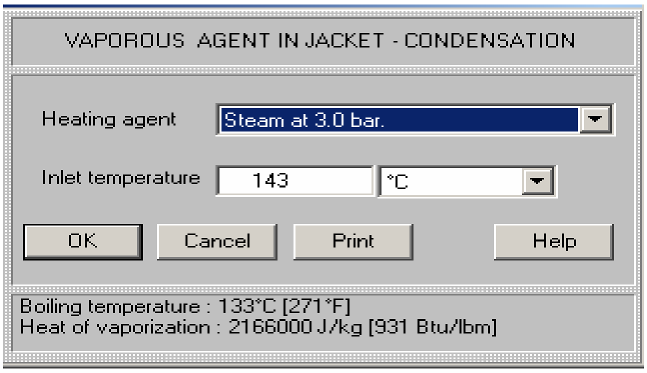
Figure 41.

NOTE:
The liquid agent velocity in inlet/outlet pipes of the jacket does not usually exceed 5 m/s.

Vaporous heating agent. Condensation in jacket

The program allows for modeling heat transfer for tanks with a number of widely used vaporous heating agents (**VA**). Choose the required **Heating agent** and the pressure (Figure 42).

The values of **Boiling temperature** and **Heat of vaporization** for the selected agent are shown at the bottom of the table. Enter the **Inlet temperature** of the selected agent in accordance with this data. If the **Lower limit of temperature** of the media you have previously entered in HEAT TRANSFER. CHEMICAL REACTION DATA AND TEMPERATURE LIMITS input table is so low as to cause freezing of the agent, VisiMix issues a message indicating that the selected agent does not correspond to the indicated range of process temperatures. In this case, select another heating agent or modify the process temperature range.



VAPOROUS AGENT IN JACKET - CONDENSATION

Heating agent: Steam at 3.0 bar.

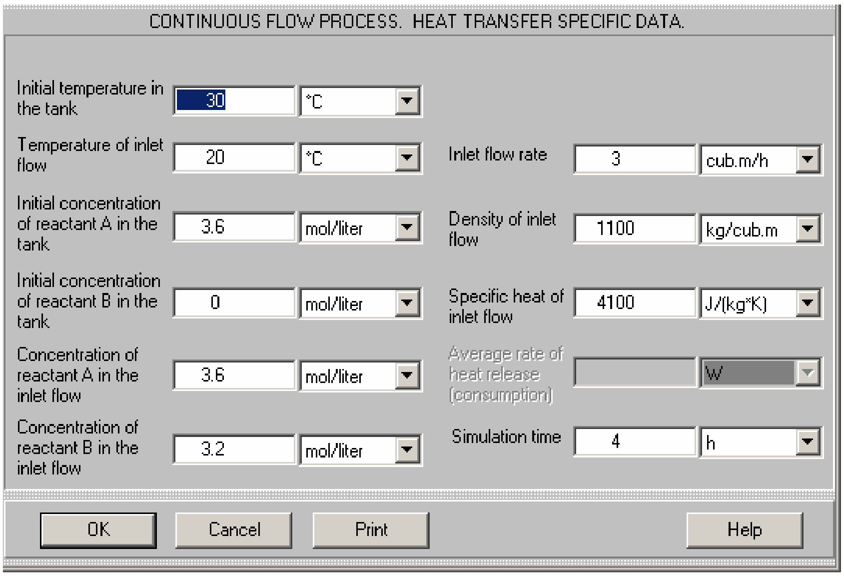
Inlet temperature: 143 °C

Boiling temperature : 133°C [271°F]
Heat of vaporization : 2166000 J/kg [931 Btu/lbm]

Figure 42.

Continuous flow process. Heat transfer specific data

The program allows for following the change in the temperature and concentrations of reactants starting from any set of initial conditions according to your input (Figure 43). All characteristics of the inlet flow, i.e. the flow rate, temperature, concentrations of reactants, and the properties are assumed to remain constant within the simulation period.



CONTINUOUS FLOW PROCESS. HEAT TRANSFER SPECIFIC DATA.

Initial temperature in the tank: 30 °C

Temperature of inlet flow: 20 °C

Initial concentration of reactant A in the tank: 3.6 mol/liter

Initial concentration of reactant B in the tank: 0 mol/liter

Concentration of reactant A in the inlet flow: 3.6 mol/liter

Concentration of reactant B in the inlet flow: 3.2 mol/liter

Inlet flow rate: 3 cub.m/h

Density of inlet flow: 1100 kg/cub.m

Specific heat of inlet flow: 4100 J/(kg*K)

Average rate of heat release (consumption): W

Simulation time: 4 h

Figure 43.

Simulation time. Enter the real time for the process stage you wish to simulate. It is recommended to start with the time equal to the mean residence time of the media in the tank determined as the quotient of the **Volume of media** by **Inlet flow rate**. The program does not perform

simulation for the **Simulation time** values greater than the tenfold value of the mean residence time. If you need to perform simulation for longer processes, use step-by-step procedure. If there are two or more inlet flows, estimate and enter average values for the sum of the flows – the total inlet flow rate, the average density and specific heat conductivity, temperature, concentrations of reactants - with respect to the parameters of each flow.
Average rate of heat release (consumption). Enter a positive number for heat release and a negative number for heat consumption.

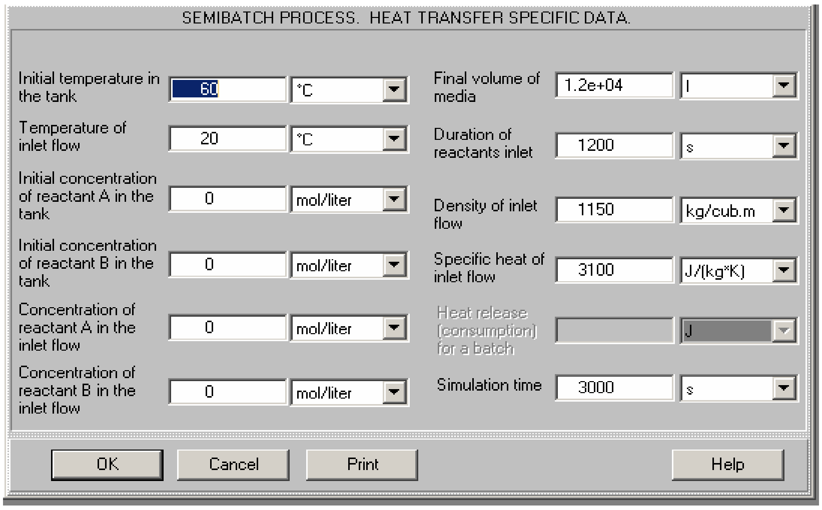
NOTE:
You must enter this parameter if you chose not to enter the data on reaction kinetics in HEAT TRANSFER. CHEMICAL REACTION AND REGIME input table.

Semibatch process. Heat transfer specific data

The data entered in this input table (Figure 44) is used for following the change in temperature and concentrations of reactants starting from any set of initial conditions. All characteristics of the inlet flow – the flow rate, temperature, concentrations of reactants, and the properties are assumed to remain constant during the time of the reactants inlet (**Duration of reactants inlet**).
Simulation time. Enter the real time for the process stage you wish to simulate. The program does not perform simulation for **Simulation time** longer than fivefold value of **Duration of reactants inlet** (i.e., for cases when the **Simulation time** value is more than 5 times greater than the **Duration of reactants inlet)**. If you need to perform simulation for longer processes, use step-by-step procedure.

If there are two or more inlet flows, estimate and enter average values for the sum of the flows – the total inlet flow rate, average density and specific heat conductivity, temperature, concentrations of reactants - with respect to the parameters of each flow.

Final volume of media. Enter the maximum volume of the media in the tank after the reagents have been injected. The **Volume of media** entered in one of the TANK input tables is regarded as the initial volume of media. The flow rate of the inlet flow is estimated by VisiMix as a ratio of the difference between the **Final volume of media** and the **Volume of media** to the **Duration of reactants inlet.**


SEMIBATCH PROCESS. HEAT TRANSFER SPECIFIC DATA.

Initial temperature in the tank	60	°C
Temperature of inlet flow	20	°C
Initial concentration of reactant A in the tank	0	mol/liter
Initial concentration of reactant B in the tank	0	mol/liter
Concentration of reactant A in the inlet flow	0	mol/liter
Concentration of reactant B in the inlet flow	0	mol/liter
Final volume of media	1.2e+04	l
Duration of reactants inlet	1200	s
Density of inlet flow	1150	kg/cub.m
Specific heat of inlet flow	3100	J/(kg*K)
Heat release (consumption) for a batch		J
Simulation time	3000	s

Figure 44.

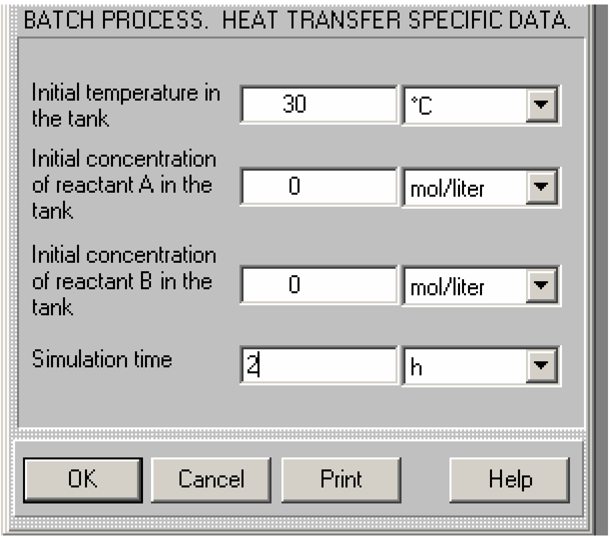
Heat release (consumption) for a batch. This is the total heat release or consumption for a batch. The entire heat is assumed to be released (or consumed) during the reactants inlet. Enter a positive number for the heat release and a negative number for the heat consumption.

NOTE:
You must enter this parameter if you chose not to enter the data on reaction kinetics in HEAT TRANSFER. CHEMICAL REACTION AND REGIME input table.

Batch process. Heat transfer specific data

The program allows for following the change in the temperature and reactants concentrations starting from any set of initial conditions according to your input (Figure 45).

Simulation time. Enter the real time for the process stage you wish to simulate.

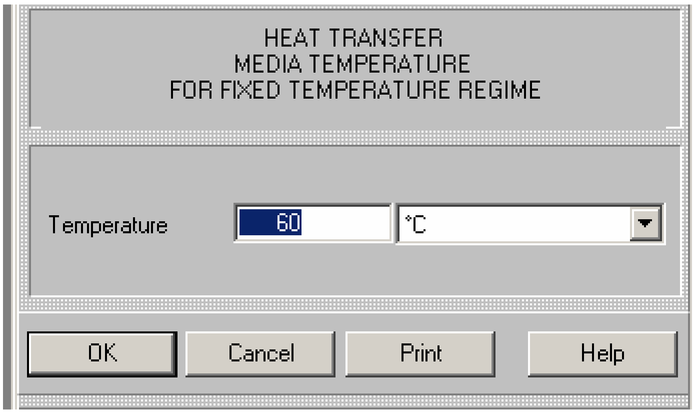

BATCH PROCESS. HEAT TRANSFER SPECIFIC DATA.

Initial temperature in the tank	30	°C
Initial concentration of reactant A in the tank	0	mol/liter
Initial concentration of reactant B in the tank	0	mol/liter
Simulation time	2	h

Figure 45.

Fixed temperature regime

Enter the **Media temperature** (Figure 46) which is the only additional parameter needed for heat transfer calculations in the **Fixed temperature regime** option.


HEAT TRANSFER
MEDIA TEMPERATURE
FOR FIXED TEMPERATURE REGIME

Temperature 60 °C

Figure 46.

SECTION 7. CALCULATION SECTIONS.

The **Calculate** menu contains all VisiMix calculation and modeling options, which are also accessible through the quick access buttons in the right screen bar. The functions accessible from the **Calculate** menu (Figure 47) help you find solutions to the main mixing-related problems.

Each of the **Calculate** submenus contains several output parameters or groups of parameters. Selecting any of these brings up the appropriate output window. If additional data is required for calculating the selected parameter, VisiMix invokes additional input tables.

A description of VisiMix TURBULENT output parameters is given in Section 8 below.

To determine the suitability of the equipment and its most important characteristics, select **Hydrodynamics**, **Main Characteristics** in the **Calculate** submenu. A table of the most important data appears. For more detailed information, turn to other options of the same submenu.

7.1. Hydrodynamics

The **Hydrodynamics** submenu is shown in Figure 47.
This option activates the mathematical simulation of hydrodynamics with respect to the design of the mixing unit and average media properties. Simulation is based on the solutions of the Reynolds equation for a turbulent flow approximated with polynomial expressions.

The conditions of unambiguity (including boundary conditions) are estimated using the equations for energy and momentum equilibrium, and practical data on mixing. In particular, experimental data on the hydraulic resistance of tanks, baffles, and blades of different geometry, and on the relations between the tangential flow and axial circulation has been used.

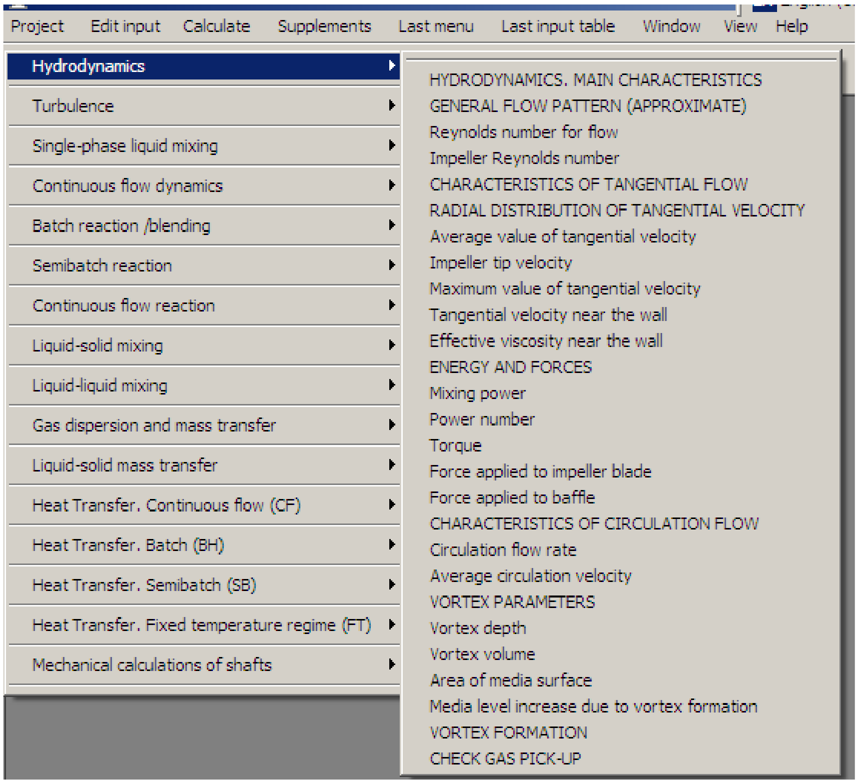


Figure 47.

7.2. Turbulence

Intensity of turbulence is evaluated in terms of rates of the turbulent dissipation of energy, which is equivalent to the local specific power per 1 kg of media. Estimations of turbulent energy dissipation rates for different parts of the volume (in vortices behind the impeller blades, in the vicinity of baffles, in the jet formed around the impeller, and so on) are based on the Kolmogoroff model of turbulence and the distribution of the flow velocities (see **Hydrodynamics**).

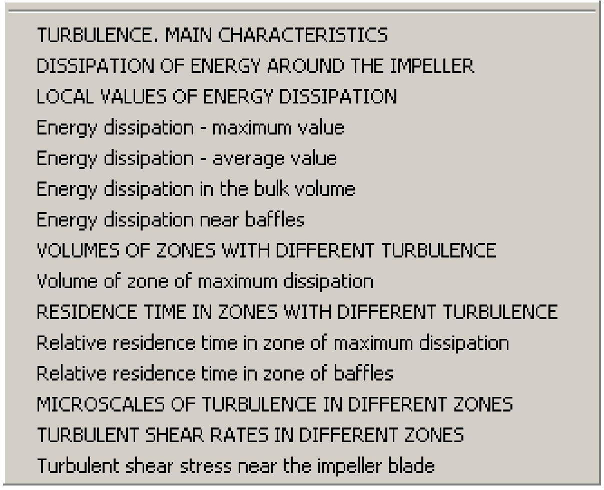


Figure 48.

NOTE:
***Turbulence parameters for Anchor and Frame impellers have never been determined experimentally*.**

7.3. Single-phase liquid mixing

Use this option (its menu is shown in Figure 49) for modeling the mixing of two liquids that are soluble in each other.

Figure 49.

This option provides a set of data for estimating the minimum mixing time required for the preparation of a uniform mixture. The simulation is based on the distribution of flow velocity (see **Hydrodynamics**) and on turbulent diffusion rate in the axial and radial directions. The mathematical models are transformed and simplified in accordance with experimental data on the general flow pattern in mixing tanks of different designs. Calculation of turbulent diffusivities is performed with respect to experimental data on macroscales of turbulent transport in mixing vessels with different impellers.
The simulation is performed for liquids with no significant difference in density and viscosity.
Mathematical modeling of volume distribution of substances is based on macroscale transport phenomena only. Micromixing phenomena are analyzed separately (See **Characteristic time of micromixing**).

7.4. Continuous flow dynamics

This option (its menu is shown in Figure 50) activates the mathematical simulation of the stimulus-response testing technique which is generally used to evaluate the reactor deviation from ideal. The testing method is based on tracing the reactor with a tracer, usually with a radioactive isotope solution. The tracer is injected in the reactor ("pulse-mode input"), and the response function curve is obtained by measuring the tracer's concentration at the outlet of the vessel.
The program calculates the response functions for different inlet and outlet positions. You can also calculate the deviation of the actual residence time distribution, RTD from RTD in an ideal ("perfect mixing") reactor of the same volume.
Physical and mathematical models of the process are basically similar to the model described in **Single-phase liquid mixing.**

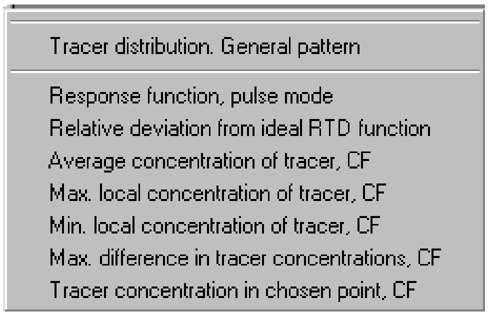


Figure 50.

This option allows for a schematic visualization of the tracer distribution in the tank. In addition, it provides a number of parameters related to the dynamics of the tracer local concentration
in any chosen point. This data can be useful for the analysis of continuous flow blending processes, as well as for the process control.

The colored area in the screen represents the tracer inlet point.

Additional data is required to determine the tracing regime. Thus, whenever you address any of the questions or parameters of this submenu for the first time, VisiMix requests additional data by invoking the input table SINGLE PHASE BLENDING. SPECIFIC PARAMETERS FOR CONTINUOUS FLOW TANK.

NOTE:
Simulation of a non-perfect mixing process may take up to 2-5 minutes; therefore please wait for the appearance of the output window.

7.5. Batch reaction/blending

This option allows for performing simulation of a “non-perfect mixing” batch reactor for a homogeneous two-component 2nd order chemical reaction A + B → C, accompanied by a parallel side reaction and the formation of a by-product. Side reactions of two types, B + B → D and B + C → D are included. The physical and mathematical models used for simulation are basically similar to the model described in **Single-phase liquid mixing**.

NOTE:
These models take into account macroscale non-uniformity in actual mixing tanks while assuming the mixing on the microscale level to be perfect. This is true if the time of micromixing (VisiMix output parameter **Characteristic time of micromixing** ***in Single-phase liquid mixing section) is considerably shorter than the characteristic reaction time.***

The modeling allows to obtain data on the distribution and change in local concentrations of reactants in a real (‘non-perfect”) reactor as a function of the reactor and impeller design. It also provides data on the formation rate and average concentration of the by-product (Figure 51) and allows for comparing the values for the selectivity of the reaction for different tank and impeller designs, mixing intensities, inlet positions, etc.

The simulation is based on the following assumptions:

a) The solution of Reactant A has been loaded into the reactor and uniformly mixed before the start of the process;
b) Reactant B or its solution is being loaded instantly, that is, the duration of loading is short compared to the mixing time;
c) The volume of Reactant B or its solution is small compared to the initial volume of the media.
d) Specific rate of the side reaction is significantly (at least 5 times) lower than specific rate of the main reaction.

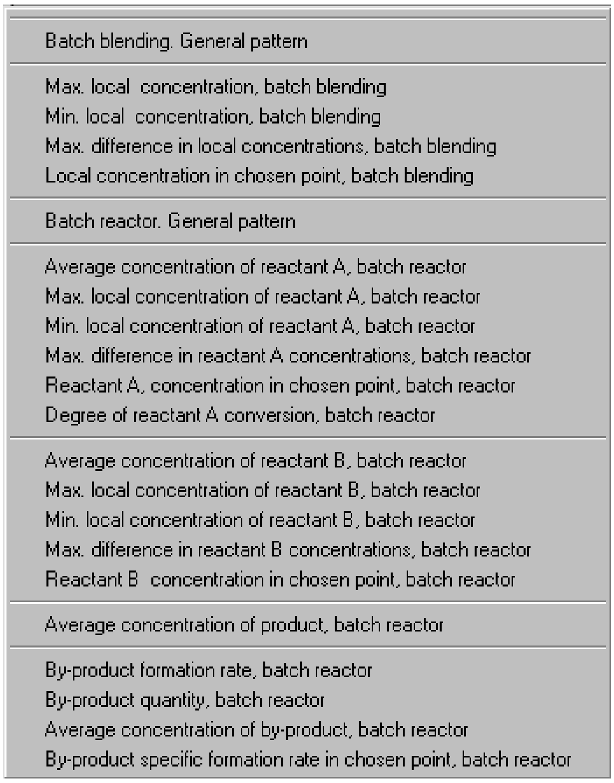


Figure 51.

The physical and mathematical models of the process are basically similar to the model described in **Single-phase liquid mixing.**

This option enables you to schematically visualize the mixing process and to evaluate the degree of non-uniformity as a function of reaction rate, quantities of reactants and inlet position. The program calculates the parameters related to both initial substances until the deviation from the "perfect mixing" conditions becomes insignificant. The concentration of the final product and the degree of conversion are calculated for the entire duration of the process.

Additional data is required for modeling a batch reaction. Thus, whenever you address any of the questions or parameters of this submenu for the first time, VisiMix requests additional data by invoking the following input tables: SINGLE-PHASE BLENDING AND REACTORS. HOMOGENEOUS CHEMICAL REACTION and INLET AND SENSOR POSITION. Supply the initial concentration for reactant A, molar quantity of reactant B, specific reaction rate and point of inlet for reactant B.

NOTE:
Whenever you return to an input table, all calculations related to the opened output windows are automatically repeated. Since simulation of "non-perfect" batch reactions may take up to 2-5 minutes, close output windows before changing initial data.

If the reaction rate for the main reaction is not known, you can evaluate the maximum possible degree of non-uniformity by entering "F" ("fast chemical reaction"). If you dispose of laboratory or practical data on the reaction, you can also estimate approximate specific reaction rate values by trial and error method. For example, start with 10 for the reaction rate and reduce it stepwise by a factor of 5-10 until the calculated reaction time estimated by the **Average concentration of product** or by the **Degree of reactant A conversion** equals a known practical value.

This submenu allows also for the simulation of batch blending. You can schematically visualize the process of admixture distribution, estimate the process duration for a desirable degree of uniformity, and select the best inlet position.

For **Blending**, supply the positions of the inlet point and point of measurement, enter “0” for specific reaction rate, and then fill in other boxes in SINGLE-PHASE BLENDING AND REACTORS. HOMOGENEOUS CHEMICAL REACTION with any positive numbers.

7.6. Semibatch reaction

This section of the program (Figure 52) allows to perform simulation of a “non-perfect mixing” semibatch reactor for a homogeneous two-component 2nd order chemical reaction A + B → C, accompanied with a parallel “side” reaction and formation of a by-product. The side reactions of two types, B + B → D and B + C → D are included. Physical and mathematical models used for simulation are basically similar to the model described in **Single-phase liquid mixing**.

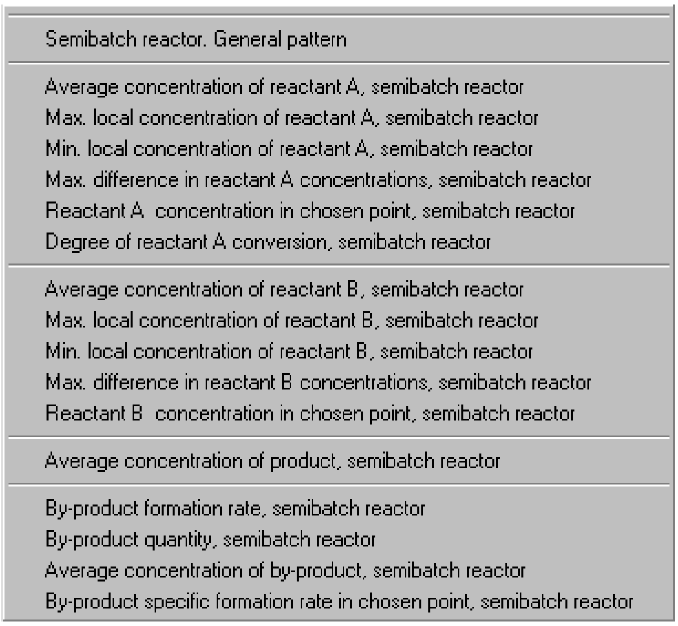


Figure 52.

NOTE:
These models take into account macroscale non-uniformity in actual mixing tanks while assuming the mixing on the microscale level to be perfect. This is true if the time of micromixing (VisiMix output parameter **Characteristic time of micromixing** ***in Single-phase liquid mixing section) is considerably shorter than the characteristic reaction time.***

The modeling allows to obtain data on the distribution and change of local concentrations of reactants in a real (‘non-perfect”) reactor as a function of the reactor and impeller design. It provides also data on formation rate and average concentration of the by-product and allows comparing selectivity of the reaction as a function of tank and impeller design, mixing intensity, inlet position, etc. Simulation is based on the following assumptions:

a) The solution of Reactant A has been loaded into the reactor and uniformly mixed before the start of the process;
b) Reactant B or its solution is not being loaded instantly. The flow rate of Reactant B or its solution is constant throughout the entire loading period;
c) The volume of Reactant B or its solution is small compared to the initial volume of the media.
d) Specific rate of the side reaction is significantly (at least 5 times) lower than specific rate of the main reaction.

The submenu allows for a schematic visualization of the mixing process and for evaluation of the degree of non-uniformity as a function of reaction rate, quantities of reactants, feed time and inlet position. Parameters related to both initial substances are calculated until the deviation from the "perfect mixing" conditions becomes insignificant. Concentration of the final product and the degree of conversion are calculated for the entire duration of the process.

Additional data is required for modeling semibatch reaction. VisiMix requests the data by invoking the appropriate input tables (see above).

NOTE:
Whenever you return to an input table, all calculations related to the open output windows are automatically repeated. Since simulation of "non-perfect" batch reactions may take up to 2-5 minutes, close output windows before changing initial data.

If the reaction rate for the main reaction is not known, you can evaluate the maximum possible degree of non-uniformity by entering "F" (fast chemical reaction), or estimate the approximate specific reaction rate by the trial and error method described in **Batch reaction/blending**.

7.7. Continuous flow reaction

This section of the program (Figures 53, 54) allows to perform simulation of a “non-perfect mixing” Continuous Flow reactor for a homogeneous two-component 2nd order chemical reaction A + B> C, accompanied with a parallel “side” reaction and formation of a by-product. The side reactions of two types, B + B> D and B + C > D are included. Physical and mathematical models used for simulation are basically similar to the model described in Single-Phase Liquid Mixing.

NOTE:
These models take into account macroscale non-uniformity in actual mixing tanks while assuming the mixing on the microscale level to be perfect. This is true if the

time of micromixing (VisiMix output parameter Characteristic time of micromixing in Single phase liquid mixing section) is considerably shorter than the characteristic reaction time.

The modeling allows to obtain data on the distribution and change of local concentrations of reactants in a real (‘non-perfect”) reactor as a function of the reactor and impeller design. It provides also data on formation rate, average and outlet concentrations of the by-product and allows comparing values for selectivity of the reaction as a function of tank and impeller design, mixing intensity, inlet position, etc.

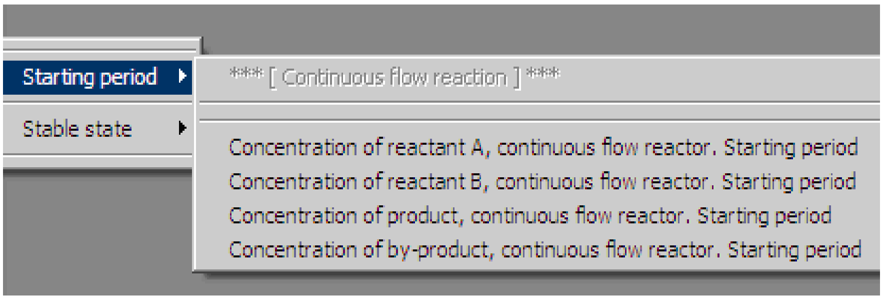


Figure 53.

Simulation of the Starting period (Figure 53) is based on ‘ Perfect mixing’ model. Starting moment (time 0) corresponds to a fully developed and stabilized mixing regime and zero concentrations of reactants and reaction products in all points of the reactor volume.

Stable state distribution of concentrations in the reactor (Figure 54) corresponds to period after Mean residence time x 10.

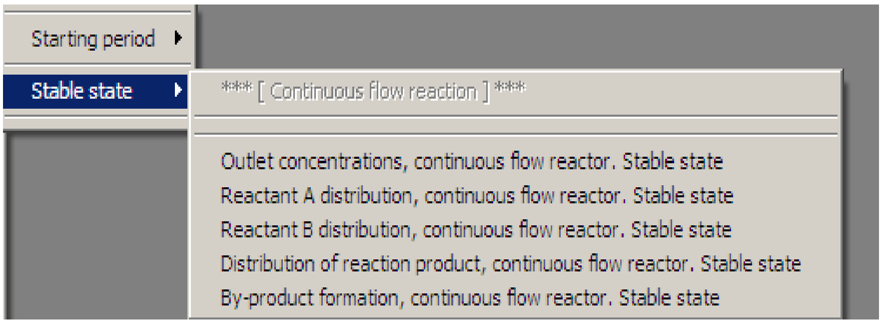


Figure 54.

If the reaction rate for the main reaction is not known, you can evaluate the maximum possible degree of non-uniformity by entering "F" (fast chemical reaction), or estimate the approximate specific reaction rate by the trial and error method described in Batch reaction/blending.

7.8. Liquid-solid mixing

Use this option (its menu is shown in Figure 53) to calculate the mixing of suspensions. The modeling of solid phase distribution is based on a diffusion model of turbulent transport in quasi- homogeneous media (see **Single-phase liquid mixing**). Separation under the effect of the rotation flow and practical data on the pick-up of particles from the bottom is also taken into account.

Additional initial data on the densities of phases, the concentration and size of particles, and the position of the outlet tube is required for modeling liquid-solid mixing. VisiMix requests this additional data whenever you address any of the questions or parameters in this submenu for the first time.

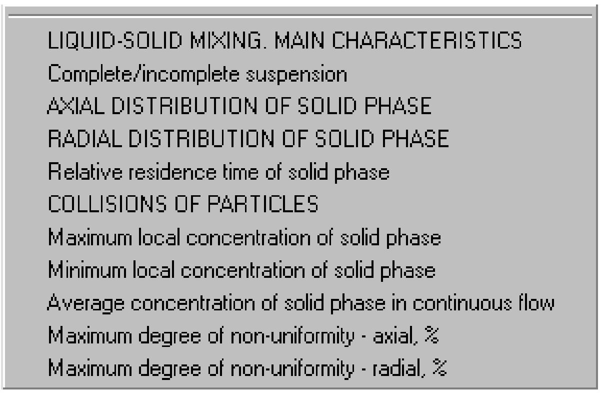


Figure 55.

Supply the data in PROPERTIES OF SOLID AND LIQUID PHASES and click OK. The program calculates average density and viscosity of the suspension and compares them with the initial input of average properties. If the difference between entered and calculated values is higher than 5%, the program issues a warning message.

When determining whether it is necessary to change your input, take into account that the hydrodynamic part of modeling, including the calculation of the **Mixing power** is based on your input of the average properties of the media.

Average density and viscosity of a two-phase system depend on the mass concentration of the solid phase in the suspension. The program calculates also the volume fraction of the solid phase. If this fraction is higher than 20%, the program issues a message informing you that the drive should have additional reservation of power. This reservation is necessary both at the start of the mixing, as the impeller may be submerged in the slurry layer, and in stable state conditions due to the increase in hydraulic resistance of the walls and bottom of the tank, as shown by recent experimental data.

NOTE:
VisiMix calculates the average viscosity of a disperse system and checks pick-up of suspension based on the assumption that there is no physical interaction between the particles.

Suitability of the equipment to a given process depends on the possibility for complete suspension of the disperse phase.

Analysis and mathematical description of flows of slurries and suspensions are based on two characteristic flow velocities: “non-settling velocity” and “washing-out velocity”. The first parameter is the minimum velocity of the suspension required for keeping the particles afloat and preventing the settling, or flotation in cases when the density of particles is lower than the density of the liquid. The second parameter is the velocity of the liquid sufficient for destroying a layer, and picking up the particles from the bottom. The “non-settling velocity” is 30-50% lower than the “washing-out velocity”.

The same approach is applied in VisiMix TURBULENT to the mixing of suspensions. The program checks if the flow velocity and turbulence in the vicinity of the bottom are high enough to satisfy each of these requirements.

If complete suspension is questionable, VisiMix issues a warning when you invoke any item in the **Liquid-Solid** menu for the first time. You may also check complete suspension directly, by clicking **Complete/incomplete suspension** in the **Liquid-Solid** menu.
The program issues an additional message explaining which of the conditions for complete suspension is not satisfied.

The message “***Partial settling is expected***” appears if the calculated velocity of the suspension is not high enough to keep the particles afloat and prevent the settling.

The message “***Complete pick-up from bottom is questionable***”
appears if the agitation starts after the solid particles have settled on the bottom, and complete suspension is questionable. In this case, too, the message that warns of possible separation of solids appears only when you ask this question for the first time.

In some cases, the calculated degree of separation of the disperse phase, in particular radial separation under the effect of rotational flow, is so great that VisiMix may deem the use of the equipment inadvisable and recommend changing the input.

If you get such a warning, you should determine whether to change the parameters of the mixing system immediately, or to proceed with the calculations.

Close all open output windows (select **Close All** from the Windows menu) before changing the data.

7.9. Liquid-liquid mixing

Use this option (its menu is shown in Figure 56) for modeling the mixing of liquids that are not soluble in each other (emulsification).

To model mixing in liquid-liquid systems, additional data on the properties of the phases must be entered. VisiMix requests this data when you address any questions or parameters in the submenu for the first time (PROPERTIES OF CONTINUOUS AND DISPERSE LIQUID PHASES input table). Calculations are based on the stochastic models for kinetics of the break-up and coalescence of drops. The modeling is performed in accordance with the distribution of local intensities of turbulence in main zones of the flow and the residence time of emulsion in these zones (see **Turbulence**).

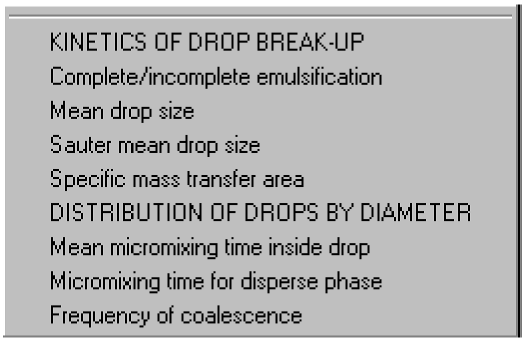


Figure 56.

Suitability of the equipment to a given process depends on the possibility for complete emulsification of the disperse phase. If complete emulsification is questionable, VisiMix issues a warning message.

Probability of coalescence depends on the repulsive pressure of the double layer on the interface, which may change considerably due to the presence of admixtures (electrolytes, coagulants, or emulsifiers). Approximate calculation of this pressure is based on the **Index of admixtures**. The program asks you to evaluate this index with respect to the composition of the liquid-liquid system.

After you enter the data and click **OK**, VisiMix calculates the average density and viscosity of the emulsion and compares them with the initial input of properties. If the difference between entered and calculated values is higher than 5%, VisiMix issues a message. When determining whether or not to change your input, take into account that the hydrodynamic part of modeling, including the calculation of the **Mixing power**, is based on your input of average properties of the media.

NOTE:
VisiMix calculates the average viscosity of a disperse system based on the assumption that there is no physical interaction between the particles.

To accelerate the solution, the simulation is performed according to a mono-disperse approximation. Calculations of drop size distributions are based on experimental data. Suitability of the equipment to a given process depends on the possibility for complete emulsification of the disperse phase. If complete emulsification is questionable, VisiMix issues a warning message.

In some cases, the calculated degree of separation of the disperse phase, in particular radial separation under the effect of the rotational flow is so great that VisiMix may deem the use of the equipment inadvisable and recommend changing the input.

7.10. Gas dispersion and mass transfer

Use this option (Figure 57) for technical calculations of bubble formation and mass transfer in gas-liquid mixing systems. The program performs mathematical modeling of distribution and breaking-up/coalescence of gas bubbles when gas is injected into the tank via a distributing device placed below the impeller.

In tanks with multistage impellers, the gas distributing device is fixed below the lower impeller. The device is often made as a perforated ring, the recommended ring diameter being about 0.5-0.9 of the impeller **Tip diameter**.
The program takes into account gas insertion from the surface, which occurs in tanks with high mixing intensity, especially if the impeller is installed close to the media surface.

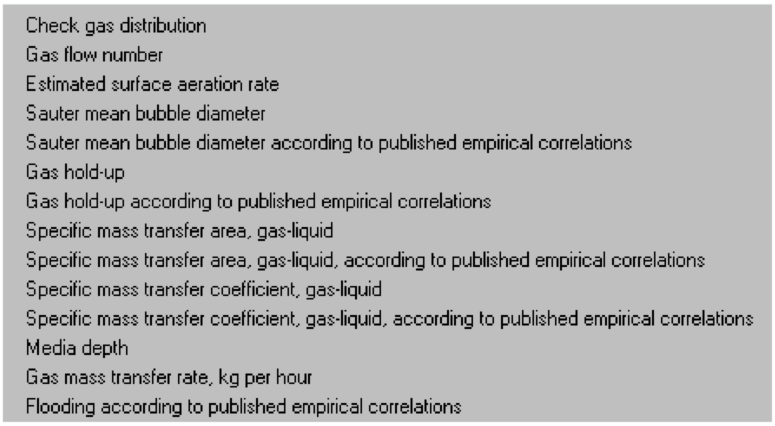


Figure 57.

The modeling is performed for baffled tanks only, because in unbaffled tanks radial separation of gas may affect the efficiency of the system. If the number of baffles or the baffle cross-section is not large enough for the efficient gas dispersion, the program issues a warning.
In addition, the impeller must be placed sufficiently close to the bottom, since otherwise the area below the impeller will not be aerated enough for the efficient operation. In multistage systems, the upper impeller must not be placed too close to the surface, since this may result in unpredictable surface aeration. In both cases, VisiMix does not perform calculations, and issues the appropriate messages.
To model gas-liquid interaction, additional data on the properties of the phases and regime parameters are required. VisiMix requests this data when you address any questions or parameters in the Gas-Liquid submenu for the first time.
Suitability of the equipment to a given process, and its efficiency depend on the complete dispersion of gas injected below the impeller, on the distribution of the bubbles across the tank cross-section, and on the transport of the bubbles downwards with the axial circulation flow. If this is questionable, VisiMix issues a warning message. If the lower impeller is fixed too far from the bottom or the flow velocity is too low to ensure satisfactory gas distribution, VisiMix issues the appropriate messages.
The gas-liquid section of VisiMix uses the results of the simulation of flow velocities, axial circulation, and turbulence performed in other VisiMix sections. The effect of the gas injection into the agitated media on these parameters is also taken into account.
Mathematical modeling is based on a set of original physical models, and on the results of numerous experimental studies. This set includes the following models:

- Radial distribution of injected gas with a radial component of flow created by impeller;
- Spontaneous surface entrainment of gas due to the effect of turbulence;
- Axial transport of gas with circulation flow and macroscale turbulent diffusivity;
- Break-up and coalescence of bubbles in the tank bulk volume;
- Mass transfer to bubbles, which are subject to deformation in a turbulent flow.

NOTE:
The models assume that bubble size corresponds to the equilibrium between break up and coalescence of bubbles in the tank bulk volume. In small vessels, and especially when gas hold-up is less than 2%, residence time of gas in liquid may not be sufficient to reach the equilibrium. Also, the mass transfer model does not take into account the "end effects", i.e. primary bubble formation.
Therefore, for small tanks the calculated mass transfer rate and mass transfer coefficients may be lower than the actual values. In industrial scale vessels, this does not happen.

It is assumed that concentration of the active component of gas or its solubility is low, and the outlet value for the volume flow rate of gas equals its inlet value. It is also assumed that local concentration of the active component in gaseous and liquid phases is the same in the entire the tank volume (perfect mixing). The composition of the gaseous mixture above the liquid surface is identical to its composition in the agitated gas-liquid mixture. Mixing tanks, under these assumptions, are used for gas-liquid mass transfer operations mainly when the mass transfer rate is limited due to the high film resistance in the liquid phase. Therefore, only the liquid phase mass transfer is taken into account, and the overall mass transfer coefficient is assumed to equal the inside (i.e. media side) film coefficient.

The model of break-up and coalescence of bubbles used in this section does not take into account the effect of surfactants, electrolytes, or other admixtures which act as inhibitors of the coalescence. Therefore, the results of the modeling correspond to the mixing in the so-called “coalescing” systems.

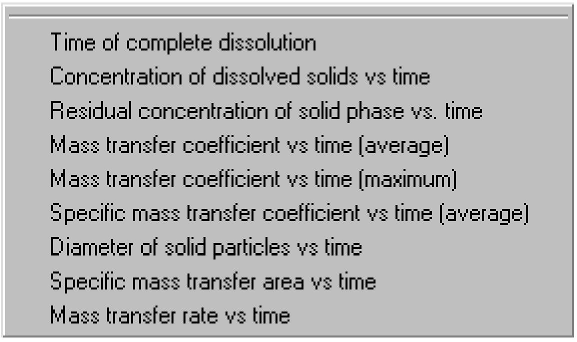
According to accumulated experimental data, mixing in gas-liquid systems is controlled by two main parameters: specific power, and superficial gas velocity. VisiMix TURBULENT calculates superficial gas velocities of up to 0.05 m/s, and calculates the specific power of up to 25 W/kg (in non-gassed conditions).

Despite a great number of experimental studies in gas-liquid mixing, the accumulated material is not representative enough for reliable conclusions regarding the physical mechanisms of the gas-liquid interaction in tanks with mechanical agitation. Therefore, VisiMix Gas dispersion section, besides the results of the mathematical modeling, provides also data based on well-known experimental correlations. In using these results, one should take into account that all the results were obtained for air-water systems, and most of them were restricted to tanks with single-stage disk turbine agitator.

7.11. Liquid-solid mass transfer

Use this option (its menu is shown in Figure 58) for modeling dissolution of the solid phase in a liquid solvent. After you have selected an item from the **Liquid-solid mass transfer** submenu, the program will request additional data by invoking the appropriate input tables (PROPERTIES OF SOLID AND LIQUID PHASES and DISSOLUTION OF SOLID PARTICLES).

VisiMix calculates the mass transfer coefficient to solid particles in a turbulent flow and simulates the dynamics of the dissolution process. It provides the calculated values of the dissolution time and graphs of main process parameters (mass transfer coefficient, concentration of the solution, the remaining concentration of the solid phase, etc.) as a function of time for a batch process.



Time of complete dissolution
Concentration of dissolved solids vs time
Residual concentration of solid phase vs. time
Mass transfer coefficient vs time (average)
Mass transfer coefficient vs time (maximum)
Specific mass transfer coefficient vs time (average)
Diameter of solid particles vs time
Specific mass transfer area vs time
Mass transfer rate vs time

Figure 58.

The simulation is based on the average (mean) particle size. It is known that the dissolution time for a real polydisperse suspension depends on the particle size distribution and is always longer than the theoretical dissolution time for a mono-disperse suspension. Therefore, the program calculates two values for the **Time of complete dissolution**: a minimum estimate calculated for particles of the average size, and a maximum estimate for the largest particles in the suspension.

The solid phase is assumed to be completely suspended in the tank, and mass transfer simulation is automatically combined with checking the complete solids suspension. If this requirement is not met the program issues an appropriate message (see **Liquid-solid mixing**). Please note that in the case of incomplete suspension (partial settling) the dissolution rate drops drastically and may become several times lower than the calculated value.

7.12. Heat transfer

7.12.1. General

VisiMix Version 2k7 TURBULENT performs two kinds of heat transfer calculations:

1. Simple calculation of heat flux and heat transfer coefficients for a fixed temperature of the media;
2. Simulation of dynamic temperature regimes of mixing tanks and reactors with respect to reaction kinetics and heat effect.

The modeling of the heat transfer includes calculating media-side heat transfer coefficients, jacket-side heat transfer coefficients and the thermal resistance of the tank wall.

Calculations of the media side heat transfer in tanks with various impellers are based on a physical model which takes into account heat transport in turbulent boundary layer and energy distribution in the flow (see **Review of Mathematical Models**).

VisiMix TURBULENT has been developed for the turbulent regime of mixing in the tank. However, for the user's convenience, Heat

transfer calculations are performed also for lower Reynolds number values.

Heat transfer in jackets is calculated using known empirical correlations, which are also referred to in the **Review of Mathematical Models**. The program calculates also the thermal resistance of the tank wall.

Heat transfer devices (HTD)

Calculations are performed for tanks with outside heat transfer devices - **conventional jackets, half-pipe coil jackets,** and **embossed/dimpled jackets**. The jacket may consist of **one** section (if there is one section only, the program regards it as "Lower") or **two** separate sections ("Lower" and "Upper").

The position of the sections, their dimensions and heat transfer areas may vary. **Lower section** may cover the tank bottom**.**

Connection of two jacket sections

The sections may be connected **"in series"** and **"in parallel"**.
Connection **in parallel:**

Liquid heat transfer agent (**LA**) inlets are placed in the lower cross-section of each section, the outlets - in the upper cross-section of each section; the inlet temperature of **LA** is the same for both sections; you should estimate and enter the flow rates for **LA**.

Condensing (vaporous) heat transfer agent **(VA)** - steam, Dowtherm vapor, etc. - inlets are placed in the upper cross-section of each section, the outlets of condensate - in the lower cross-section of each section; the inlet temperature and pressure of **VA** are the same for both sections.

Connection **in series:**

Liquid heat transfer agent (**LA**) inlet is placed in the lower cross-section of the lower section; **LA** outlet is placed in the upper cross-section of the lower section; the inlet of the upper section placed in its lower cross-section is connected to the outlet of the lower section; the outlet of the **LA** is placed in the upper cross-section of the upper jacket section. The flow rate of **LA** is the same in both jacket sections. Enter the inlet temperature of **LA** for the lower section; the inlet temperature for the upper section is assumed to be equal to the temperature of **LA** at the outlet of the lower section.

Condensing (vaporous) heat transfer agent **(VA)** - steam, Dowtherm vapor, etc. - inlets are placed in the upper cross-section of the upper section, the outlet of condensate and steam (vapor) of the upper section is placed in its lower cross-section and connected to the inlet pipe placed in the upper cross-section of the lower section. The outlet of condensate is placed in the lower cross-section of the lower section. The steam (vapor) pressure in both sections is assumed to be the same, the inlet temperature for the lower section is assumed to be equal to the saturation temperature.

Heat transfer agents (HTA)

The program performs calculations of heat transfer in heat transfer devices for two kinds of HTA - liquid agents (**LA**) and condensing steam or organic vapors (**VA**). There is no need to enter the physical properties of heat transfer agents: you must only select an appropriate agent and enter the inlet conditions: the inlet temperature for **LA**, the inlet temperature and pressure for **VA**. The required properties of heat transfer agents are retrieved by the program from its database. The program includes also subprograms for approximate calculations of temperature-dependent physical properties of heat transfer agents.

Properties

Simulation of temperature regimes is performed with respect to the change in physical properties of liquids (the media and **HTA**) as a function of the temperature. For this purpose, the program includes algorithms and sub-programs for approximate calculations of temperature functions of the density, viscosity, specific heat and heat conductivity of liquids, which are based on a single value of the property and the corresponding temperature. The calculation methods for the viscosity and specific heat capacity are similar to the graphical method proposed by Lewis, W. K. and L. Squires for viscosity (see J. Perry, Chemical Engineering Handbook,
pp. 3-281,282, Fig. 3-50). Different functions are used for water solutions and organic substances. You will therefore be asked to specify the media in addition to the values of the properties.

NOTE:
The methods for calculating physical properties are approximate. Their accuracy is sufficient for heat transfer calculations, but they are not recommended for general use. The table of properties of the most frequently used water solutions and organic solvents is accessible through HEAT TRANSFER PROPERTIES OF THE MEDIA input table. It will help you to approximately estimate the initial data for heat transfer calculations.

Process regimes. General information

The main menu includes three Heat Transfer options related to the main process regimes - Continuous flow (**CF**), Batch (**BH**) and Semibatch (**SB**). Each of them includes two submenus according to the type of the heat-transfer agent and the process in the heating/cooling device (HTD). The **Liquid agent (LA)** option is used to calculate heating or cooling in the tank with a liquid heating agent (LA). The heat transfer mechanism may correspond to free convection or forced convection in laminar or turbulent flow conditions. In the course of the simulation, the program estimates the flow and heat transfer regime and selects the appropriate correlation.

Before starting the simulation by selecting a parameter in the corresponding submenu of Heat Transfer options of **Calculate**, you will be asked to fill in the appropriate input tables of initial data according to a particular mixing case. However, for all process regimes it is necessary to enter the **Lower and Upper limits of temperature** of the media in the tank in order to define the range for the simulation. It is also necessary to enter the **Simulation time.**

If the calculated temperature (**Media temperature**) falls outside the prescribed temperature limits, the program stops calculation and issues an appropriate message, indicating the time when this occurs. To obtain more information about the process, enter a new value for the **Simulation time,** which must be lower than the one indicated in the message in the corresponding HEAT TRANSFER. SPECIFIC DATA input table for CF, BH and SB processes.

The results obtained with heat transfer calculation options are displayed mainly as graphs; the parameter you selected is presented as a function of time within the simulation period**.** To present graphs as tables, use the **Report** option.

The simulation is based on the common equations of heat equilibrium with respect to heat capacity of the media and the tank. You select the tank material in TANK SHELL CHARACTERISTICS input table, and the properties of the material will be retrieved from the VisiMix database. You may enter the tank mass according to the tank drawings. If the exact mass is not known, VisiMix calculates it.

Chemical reaction with heat release or consumption

The program simulates simple heating or cooling in tanks, and also temperature regimes of chemical reactors. Calculations are performed with respect to a second-order single-phase chemical reaction:

$$\mathbf{A + B} \rightarrow \mathbf{C} + Q_r\,,$$

where Q_r is the specific heat release/consumption of the process.
You may enter kinetic data and heat effect of the reaction in the HEAT TRANSFER. CHEMICAL REACTION DATA AND TEMPERATURE LIMITS input table. The heat release is calculated as a function of the current concentrations and temperature according to the Arrhenius equation. If the kinetic and thermodynamic constants for the reaction are not available, the program may perform calculations based on the average heat release/consumption value you entered. This option may also be useful for simulating temperature regimes of heterogeneous reactions with total heat release value based on experimental data.

7.12.2. Modeling of temperature regimes

VisiMix allows you to perform heat transfer calculations for the following types of processes: Continuous Flow (**CF**), Batch (**BH**), Semibatch (**SB**), and for Fixed temperature regime (**FT**). For each of these processes you may perform simulation for the case of liquid heat transfer agent (**LA**) in jacket, and for the case of vaporous heat transfer agent (**VA**) in jacket. The menu of one of the **Heat Transfer** options in **Calculate** is shown in Figure 59.

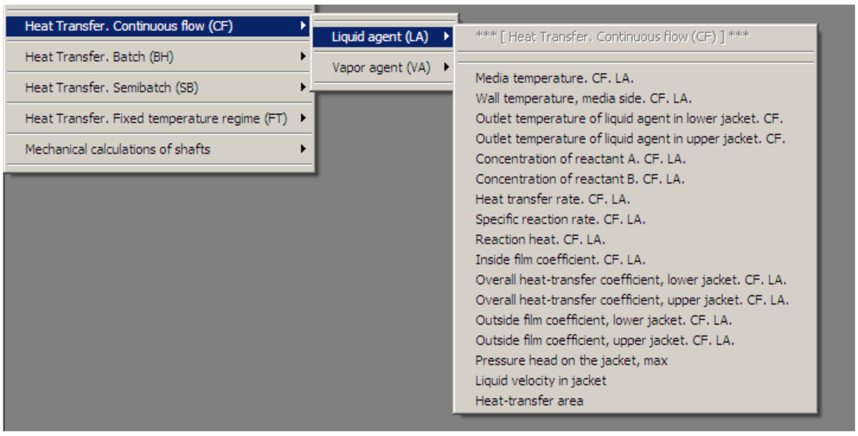


Figure 59.

Continuous flow process - CF

This option provides mathematical modeling of the dynamics of a continuous flow mixing tank with a heat transfer device. The process eventually reaches a steady-state regime. Granted the sufficient simulation time, the final results obtained in the simulation will represent the steady-state parameters.

In this case, the **Heat transfer area** in the tank is assumed to be constant and is calculated according to the **Volume** or **Level of media** in the tank.

You select a starting point of the simulation, i.e. the media temperature and the concentrations of the reactants. The simulation, including the simulation of transition regimes, can be started from any reactor state.

Batch process - BH

This option provides mathematical modeling for Batch heating/cooling of the tank or Batch chemical reactor with a heat transfer device. In this case, the **Heat transfer area** in the tank is assumed to be constant and is calculated according to the **Volume** or **Level of media** in the tank.

In the case of a chemical reaction, both reactants are supposed to be loaded and distributed in the reactor before the simulation starts.

Semibatch process - SB

This option provides mathematical modeling of Semibatch reactors with heat transfer devices. It is assumed that the solution of reactants A and B is loaded into the tank in the beginning of the process. The volume of the solution is the minimum volume of the media in the tank and corresponds to the value of **Volume of media** you entered in the TANK input table. At moment “0”, the loading of the solution of reactants A and B into the tank begins. The solution is loaded at a constant flow rate until the volume of the media becomes equal to the **Final volume of media** you entered in the SEMIBATCH PROCESS. HEAT TRANSFER SPECIFIC DATA input table. You must also specify the **Duration of reactants inlet**, **Density, Specific heat capacity** and **Temperature of inlet flow**. The volume flow rate of the inlet flow during the inlet period is calculated as:
(Final volume of media - Volume of media) / Duration of reactants inlet .
The current values of the **Volume of media** in the tank and of the **Heat-transfer area** of heat transfer devices are calculated as functions of time and with respect to the flow rate of the inlet flow.

If kinetic data and **Heat effect of reaction** have been previously entered, VisiMix calculates heat release with respect to the current concentrations of the reactants and temperature. If the **Heat release/consumption for a batch** was entered instead of the **Heat effect of reaction**, the reaction heat release (consumption) is assumed to be constant during the reactants inlet, and to become **zero** after the end of the inlet period.

Fixed temperature regime - FT

This option allows for performing common heat transfer calculations of the tank for a given single set of conditions, i.e. the volume and temperature of the media. No additional data on the process, such as reaction kinetics or heat release, are necessary. All program output in this case is given in the form of tables.

Fixed temperature calculations are the most simple and fast of all VisiMix Heat Transfer modeling options. You may use this option not only for calculating steady-state heat transfer rates for fixed conditions, but also in combination with one of the simulation options as the first stage for a preliminary selection of the equipment, the heat transfer agent, its inlet temperature and flow rate, etc. Another possible application is obtaining output parameters for any desired point on the process simulation curves by reading the **Media temperature** at this time coordinate from the graph **Media temperature vs. time,** and entering it in the FIXED TEMPERATURE. HEAT TRANSFER SPECIFIC DATA input table**.**

7.13. Mechanical calculations of shafts

Use this option (its menu is shown in Figure 60) to perform the mechanical calculations required for checking the shaft reliability. The program includes calculations for the critical frequency of shaft vibrations and maximum stresses in dangerous cross-sections. Calculations are based on the shaft sizes as preliminarily estimated and entered by you. If the results of the calculations are negative, the program issues appropriate messages. In this case, you should modify your input, e.g., increase the cross-section of the shaft section mentioned in the message, or reduce the number of revolutions, etc.

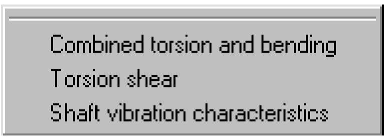


Figure 60.

The impeller (for multistage systems - all impellers) is assumed to be submerged in the liquid so that the central vortex (see **Hydrodynamics, Vortex depth**) does not reach the impeller. The maximum torque of the impeller drive you selected is also used as initial data. Therefore, the mechanical calculations are always performed after the calculations of the hydrodynamic parameters. The program automatically performs two preliminary checks, selecting the drive (power of the drive must be high enough for the selected mixing system) and the vortex depth. If either the impeller or the drive do not correspond to the requirements described above, the program issues appropriate messages.

Shaft types

The calculation methods used in the program are related to the vertical console metal shafts with stiff fixation of the upper end in bearings. The following types of shafts are considered:
1) A solid stiff shaft with a constant diameter (**single-diameter shaft**, or **regular**);
2) A stiff shaft consisting of two parts, either both solid, or the upper solid stage and the lower hollow (tubular) stage with different diameters (**variable diameter shaft**, or **combined**);

Both shaft sections are supposed to be made of materials with identical mechanical properties. A built-up shaft with stiff couplings is regarded as a single item.

The term “stiff shaft” means that the rotational speed of the shaft is lower than the shaft’s critical (natural) frequency of vibrations. Calculations are performed for shafts with one, two and three identical impellers, which are assumed to be fixed on the same section of the shaft (see diagrams in the SHAFT DESIGN input table).

Calculations can also be performed for glass-lined shafts and shafts with other coatings. However, applicability of the VisiMix suitability criteria is not guaranteed for these cases.

Calculated parameters and suitability criteria

The program performs three sets of calculations:

Maximum torsional shear stress. The torque applied to the shaft is assumed to correspond to the maximum value of the driving momentum due to motor acceleration, i.e. 2.5 times higher than the motor rated torque. These calculations are performed for the upper cross-sections of the upper and lower stages of the shaft. A single-stage shaft (regular) is regarded as the upper stage of a 2-stage shaft with a zero length for the lower stage. The shaft is considered to be strong enough if the calculated stress value is equal or higher than 0.577 of the yield strength of the shaft material.

Combined torsion and bending. The shaft is assumed to be occasionally exposed to uneven bending force applied to one of the impeller blades. The maximum combined stress is calculated using the EEUA method. These calculations are performed for the upper cross-sections of the upper and lower shaft sections. A single-stage shaft (regular) is regarded as an Upper stage of a 2-stage shaft with a zero length for the lower stage. The shaft is considered to be strong enough if the calculated stress value is equal or higher than the yield strength of the material.

Critical frequency of vibrations. The shaft is considered to be stiff if the rotational speed is less than 70% of the calculated critical (natural) frequency. According to many years' practical experience, this condition is fully reliable for mixing in homogeneous liquids, as well as in liquid-liquid and liquid-solid systems. For gas-liquid systems, the impeller rotational speed must be about 60% of the critical frequency. To avoid additional sources of vibrations, two more conditions are recommended:

1) The product of the rotational speed of the shaft and the number of blades must not equal the critical (natural) frequency of the shaft, and
2) The number of baffles in the tank must not be equal to the number of impeller's blades. In tanks with an even number of baffles, it is advisable to use impellers with an odd number of blades.

7.14. Supplement. Tanks with Scraper agitators.

Scraper agitators are used in tanks and reactors that require intensive heat transfer to a jacket. Their application is typical the cases when it is necessary to prevent adhesion of solid particles (for instance, in crystallizers, in reactors for precipitation processes, for suspension polymerization, etc.) or formation of a high viscosity film on the heat transfer surface of the tank. Some kind of plastic, in the most cases -Teflon, is used as a material for the scrapers. The close contact of the scrapers to the tank wall is ensured due to flexibility of the plastic.

The scrapers are fixed to horizontal hands. Accordingly to the calculations and experimental results, in mixers of technically reasonable design influence of the hands on mixing is negligible. It can be checked by comparing of the power values calculated for scrapers and for horizontal hands without scrapers

Intensive heat transfer to the tank wall that is swept with scrapers occurs due to periodic replacement of a boundary liquid film that is in thermal equilibrium with the wall (Tfilm = Twall) by a 'new' layer with different temperature. If turbulent mixing in the tank is intensive enough, this temperature is equal or nearly equal to the average temperature of the media. Calculation of Media-side heat transfer coefficients for such conditions is based on the well known theoretical solution for non-stationary heat conductivity in a semi-infinite body. Close to the lower limit of turbulent regime the radial turbulent mixing between periphery and bulk part of the tank volume is not so good, and it results in decrease of the heat transfer rate.

NOTE:
Even small distance between the scraper and the tank wall can cause a significant reduction of heat transfer rate.

Entering initial data for a new Project.

- Enter the **Project** name and select a Tank as described in par. **5.1** and **6.1**.
- Select '**No baffle'** option in the **Baffle selection** table.
- After obtaining agitator selection table click '**Cancel**'.
- Enter Average properties of media as described in par. 6.5.1.
- Select **Supplements> Scraper agitators>Scraper agitator. INPUT** and fill the input table
- Select and click the menu options corresponding to the purpose of calculations.

If you select **Heat transfer** option for the first time, the program will display a table for input of **Heat transfer properties of media.**

Editing the initial data.

Editing of the initial data for **Supplements** is performed using the Menu icon **Initial Data explorer**. The **Last input** table option can be also used.

Returning from Supplements to the main part of the program.

In order to return from **Supplements** to the main part of the program click **EXIT** in the **Supplements-Scraper agitators** menu.

NOTE: The Scraper agitators can be used only in tanks without baffles. If the Supplement is used for an existing Project that includes a tank with any type of baffles, a corresponding message arrives on the screen. If it happens, you have to return to the main program and select the No baffles conditions.

SECTION 8. OUTPUT PARAMETERS

8.1. Hydrodynamics

8.1.1. General flow pattern

The visualization is based on the results of approximate modeling the flow with stabilized hydrodynamics. It imitates the motion of tracer particles, which have been injected at random into the tank. The time that has elapsed since loading the tracer particles is displayed on the screen.

8.1.2. Reynolds number for flow

This value is based on the average velocity of the flow and radius of the tank. The lower limit of a turbulent regime corresponds to the Reynolds number value of about 1500. Significant changes in hydrodynamics are observed when the Reynolds number value is lower than 1000. The current version of VisiMix does not perform calculations for Reynolds number values lower than 1500.

8.1.3. Impeller Reynolds number

This is a traditional definition of the Reynolds criterion. It is calculated by a common formula as the product of rotational velocity and tip diameter of impeller divided by kinematic viscosity.

8.1.4. Impeller tip velocity

This parameter represents the speed of the outer edge of the impeller blade. It is used for comparing the blade velocity and the velocity of the media flow.

8.1.5.Characteristics of tangential flow

Radial distribution of tangential velocity.

This parameter represents the height average radial profile of tangential velocity. Numerous measurements have shown that in a well developed turbulent flow, local profile of tangential velocity is close to the average at almost any height, except for the impeller area.

Average value of tangential velocity

This parameter represents the volume average value for tangential velocity.

Maximum value of tangential velocity

This is the maximum value on the tangential velocity profile, see **Radial distribution of tangential velocity**.

Tangential velocity near the wall

This is the average tangential velocity near the wall outside the boundary layer. Velocity degradation in the boundary layer is beyond the scope of VisiMix modeling.

8.1.6. Effective viscosity near the wall

For non-Newtonian media, this parameter depends on the value of shear rate in the boundary layer on the tank wall. Calculation of the shear rate is based on the results of modeling the flow velocity distribution.

8.1.7. Mixing power

This parameter is calculated for stable state mixing. The calculation is based on the results of mathematical modeling of velocity distribution and on experimental resistance factor values for blades of different configurations. Here data on average density and viscosity, which have been previously entered into the system, are used. If the calculated mixing power exceeds 70% of the motor power rating you have previously entered into the system, the warning ***"Mixing power is too high for your drive"*** is issued.

The 30% reservation accepted in VisiMix is based on practical experience. It takes into account usual level of energy losses in electric drives with mechanical speed reducers (gyres). If the speed reduction is performed using electrical or electronic speed control devices, selection of the motor power has to be based on the rated torque moment of the low speed shaft that must be included in the technical characteristic of the drive. The recommended 30% reservation in this case must be related to the calculated **Torque** value.

8.1.8. Power number

This parameter represents the *Np* coefficient in the equation

$$P = N_p \rho n^3 d^5$$

where

P is the mixing power, W;

ρ is average density of the media, kg/cub. m;

n is rotational speed, 1/s; and

d is impeller diameter, m.

VisiMix first calculates the mixing power by solving hydrodynamic equations, and then *Np* is calculated using the formula given above.

Torque

This parameter represents the value for the torque imparted by the rotating impeller to the media.

Force applied to impeller blade

This parameter represents the resultant of the forces applied to the blade by the flow.

Force applied to baffle

This parameter represents the resultant of the forces applied to the baffle by the flow.

8.1.9. Characteristics of circulation flow

Circulation flow rate

This parameter is calculated as the sum of circulation flow rates in all main circulation loops in the vessel. See also **General flow pattern**.

Mean period of circulation

The average time of a single cycle of media circulation is calculated on the basis of the **Circulation flow rate**. In many cases, it is recommended to reduce this parameter, for instance, to avoid significant change in concentration near the inlet pipe. To reduce circulation time without increasing the mixing power, try an impeller with a larger tip diameter and lower pitch angle of blades.

Average circulation velocity

This is a value of axial velocity defined as average over the tank volume.

8.1.10. Vortex formation

This diagram shows form of the vortex in your mixing tank.
The phenomenon of vortex formation is mainly significant for unbaffled tanks. In baffled tanks, the vortex is usually small and can be disregarded. However, at high RPM values, the vortex may be quite large. It is often unstable, and its height and shape may change considerably in the course of the process. In these cases, calculated vortex parameters should be regarded as estimates only.

Vortex depth

If the vortex is too deep and reaches the impeller, unstable gas caverns may form around the impeller blades. The resulting shaft vibrations may reduce the reliability of the equipment. Gas insertion into the media may also occur. VisiMix lets you know if such conditions are expected.

Vortex volume

This value must be taken into account in the continuous flow processes for calculating mean residence time of media.

Media level increase due to vortex formation

Due to vortex, there is an increase in the level of media near the tank wall. In some cases, this may cause media overflow. In addition, it may increase the heat transfer area in cases of heating/cooling in jacketed tanks.

Area of media surface

This is the area of the media surface, calculated with respect to deformation of surface due to vortex formation.

8.1.11. Check gas pick-up.

High turbulence close to the surface or big vortex width in the impeller depth can result in a significant insertion of gas into agitated liquid. Sometimes this phenomenon is not desirable – it causes flotation of particles, or oxidation of the reactants and reaction products, etc.
In order to perform simulation of the surface pick-up of gas, the program will ask you to enter data on Surface tension (Figure 34).

8.2. Turbulence

8.2.1. Local values of energy dissipation

The entire mixing volume is assumed to be divided into zones - the zone behind the impeller blade, the zone behind the baffles, the jet around the impeller, and the bulk volume. This table provides estimates for the energy dissipation values in these main zones.

Non-uniform distribution of energy dissipation is important for micro-mixing, emulsification, and crystallization. A high degree of non-uniformity has a positive effect on emulsification and a negative effect on crystallization. For single-phase mixing and suspension processes, a more uniform distribution of energy is preferable. To reduce the degree of non-uniformity, try reducing the pitch angle of the blades or the number of baffles.

NOTE*:*
For Anchor and Frame impellers, these values have never been determined experimentally.

Energy dissipation - average value

This parameter represents the volume average specific power, and is calculated as the mixing power per kg of media.

Energy dissipation - maximum value

This parameter is calculated as an average value of the turbulent dissipation rate in the zone with the highest degree of turbulization. In most cases, it takes place in the vortices formed behind the impeller blades. Energy dissipation in this area depends on the difference between the impeller tip velocity and the tangential velocity of the media. The most important microscale phenomena, such as drop break-up, breaking of crystals, nucleation, and efficient micro mixing take place in these zones.

NOTE:
For Anchor and Frame impellers, this value has never been determined experimentally.

Energy dissipation near baffles

This parameter represents a characteristic value of energy dissipation behind the baffles calculated using the velocity of the flow past the baffles. If this value is smaller than energy dissipation in the bulk volume, the value for the bulk volume is given.

Energy dissipation in the bulk volume

This value controls micro-mixing in single-phase reactors. To increase this value without increasing the mixing power, reduce the pitch angle of the blades or the number or width of the baffles; alternatively, increase the tip diameter of the impeller and reduce the number of revolutions.

Dissipation of energy around the impeller

A jet forms around the impeller. Turbulent dissipation in this jet, at least near the impeller, is relatively high, which helps achieve better micro-mixing. Its influence on drop breaking is negative because of coalescence.

NOTE:
For Anchor and Frame impellers, this value has never been determined experimentally.

8.2.2. Volumes of zones with different turbulence

Volume of zone of maximum dissipation

This parameter represents and estimate of the volume in which the energy dissipation is close to the maximum value for energy dissipation calculated by VisiMix. Despite the fact that the energy dissipation behind the impeller blade may be much greater than the average, the volume of this zone may be small compared to the total mixing volume.

Volume of zone surrounding baffles

This parameter represents characteristic volume of the zone behind the baffles, in which the energy dissipation may differ significantly of the energy dissipation in the bulk volume, see also **Local values of energy dissipation**.

Characteristic time of micromixing

This parameter represents the time for the degradation of microscale concentration non-homogeneity, and it must be taken into account in the analysis of fast chemical reactions.

8.2.3. Residence time in zones with different turbulence

This table provides the relative residence time values for the zone of maximum energy dissipation, the zone behind the baffles, and tank bulk volume. These values are calculated as the ratio of the volume of the respective zone to the total mixing volume.

8.2.4. Microscales of turbulence in different zones

Estimation of microscales of turbulence is based on Kolmogoroff hypothesis. The minimum value of a microscale corresponds to the maximum energy dissipation. This value is important for drop breaking and coalescence. The microscale value corresponding to the tank bulk volume is in control of micromixing time in Single-phase liquid mixing.

8.2.5. Turbulent shear rates in different zones

The following formula is used by VisiMix for calculation of the average shear rate and local shear rates around the agitator, in the tank bulk volume and near the baffles:

$$\Gamma_{turb} = (\varepsilon / \nu)^{1/2},$$

where:

Γ_{turb} is the turbulent shear rate, 1/s
ε is the turbulent dissipation rate (near the agitator blade, near the baffle, or in the tank bulk volume, respectively), W/kg or m^2/s^3, and
ν is the kinematic viscosity of liquid media, m^2/s.

The physical meaning of Γ_{turb} variable is the ratio of turbulent fluctuation velocity V_0' at the Kolmogoroff scale, δ_0, (internal scale of turbulence) to the value of δ_0:

$$\Gamma_{turb} = V_0' / \delta_0$$

This parameter must not be confused with average velocity gradient, and its value is typically one or two orders of magnitude greater than the latter. The turbulent shear rate, Γ_{turb} is the characteristic shear rate at the microscale level that governs such processes as mass transport to growing and from dissolving solid particles.

8.2.6. Turbulent shear stress near the impeller blade

This parameter represents microscale characteristics of internal friction values. It is connected to the turbulent shear rate, Γ_{turb}
by the equation

$$\tau_{turb} = \mu\Gamma_{turb},$$

where μ is dynamic viscosity of the media.

8.2.7. Characteristic time of micromixing. See par.8.3.3.

8.3. Single-phase liquid mixing

8.3.1. Macromixing time

This parameter characterizes the time required for the distribution of solute (admixture, tracer, paint, etc.) throughout the entire volume of the tank. It is calculated as the time required to reduce the maximum difference of local concentrations of the admixture to about 1% of its final average value (in batch mixing conditions). The admixture is assumed to be injected instantly. Selection of the real duration of blending is based on the sum of **Macromixing time** and the **Characteristic time of micromixing**.

To reduce the macromixing time in an unbaffled tank, try increasing impeller tip diameter or pitch angle of the blades. In baffled tanks, reducing the macromixing time is usually achieved by increasing the mixing power.

8.3.2. Mean period of circulation

The average time of a single cycle of media circulation is calculated on the basis of the circulation flow rate. In many cases, it is recommended to reduce this parameter, for instance, to avoid significant change of concentration near the inlet pipe. To reduce circulation time without increasing the mixing power, try an impeller with a larger tip diameter and lower pitch angle of blades. This parameter is also calculated in **Hydrodynamics** section.

8.3.3. Characteristic time of micromixing

This parameter represents an estimate of the time required to achieve uniform distribution of the dissolved substances down to the molecular level. It is assumed to depend on the molecular diffusion of solute, while the scale of mixing due to molecular diffusion only is supposed to correspond to the microscale of turbulence. Micromixing time is estimated both as the diffusion time, and as the maximum lifetime of a volume element, which has elapsed before the element enters the zone of the maximum dissipation rate. The final value of this parameter is calculated with respect to both estimates. Characteristic size of the volume element is assumed equal to the microscale of turbulence in the tank bulk volume.

8.4. Continuous flow dynamics

8.4.1. Tracer distribution. General pattern

Visualization of the tracer distribution helps choosing optimal inlet/outlet and sensor positions for the process control.

8.4.2. Response function, pulse mode

This parameter is important for automatic control of reactors. The results of the mathematical simulation of the reactor’s dynamic characteristics are presented in the form of stimulus-response functions for a pulse type of tracer input signal. To calculate the response function, enter the coordinates of the inlet point.

8.4.3. Relative deviation from ideal RTD function

Residence time distribution (RTD) is used as a basis for the analysis and mathematical modeling of "non-ideal" reactors ("non-perfect" mixing). It is calculated as an integral of the Response function. For an ideal ("perfect mixing") reactor, RTD corresponds to an exponential function. Significant deviations from this function are observed at the beginning stage of the process. They characterize the degree of deviation from ideal and can be important for the process control. To shorten this stage, try increasing the **Circulation flow rate** or decreasing the mixing time. You can also reduce the deviation by selecting optimal positions of inlet and outlet points.

8.4.4. Average concentration of tracer in CF tank

The form of the curve for the average concentration of tracer in continuous flow tank differs from exponential which is characteristic for "perfect mixing" reactor when the residence time value is comparable to the **Macromixing time**.

8.4.5. Maximum difference in tracer concentrations, CF.

These parameters determine the tracer distribution as a function of mixing device and inlet position. They can be used to analyze and improve single-phase mixing.

8.4.6. Local concentrations of tracer, CF
Max. local concentration of tracer, CF
Min. local concentration of tracer, CF

These graphs illustrate degree of 'non-ideality' of the reactor from the point of mixing and distribution of tracer. Along with the maximum and the minimum concentration values, it is possible to get graphs of local concentration in any point of the tank by corresponding positioning of the sensor (see 8.4.7)

8.4.7. Tracer concentration in a chosen point, CF.

The position of the virtual sensor in the tank is specified in the input table SINGLE-PHASE BLENDING **&** REACTORS. SENSOR POSITION. The sensor measures the concentration of the tracer in this specified point, and the local concentration in this point as a function of time is shown in the graph.

8.5. Batch reaction/blending

8.5.1. Batch reactor. General pattern

The program provides simultaneous visualization of both reactants' distribution in the tank. Use visualization to select optimal inlet point for reactant B.

8.5.2. Average concentration of reactant A and B, batch reactor

In "perfect mixing" reactors, the form of the curve of average concentrations of reactants depends only on their initial concentrations in the reactor, the reaction equation and kinetic constants. In actual mixing conditions, the form of the curve of average concentrations depends also on the inlet location and the design of the mixing unit.

8.5.3. Maximum difference in local concentrations, batch reactor

The changes in the degree of non-uniformity of distribution of local concentration values help analyze the course of the process, especially at the start when concentration of reactant B is relatively high. For some reactions, considerable differences of local concentrations and long non-uniformity periods can lead to formation of by-products and decrease the product yield. These effects can be reduced by decreasing the **Macromixing time**, and sometimes by choosing better inlet positions. The data on the distribution of local concentrations can be used also for choosing sensor position in the reactor.

These parameters are calculated for the beginning stage only, until the difference of local concentration values becomes insignificant.

8.5.4. Local concentration in chosen point (batch blending and batch reactor)

The position of the virtual sensor in the tank is specified in the input table SINGLE-PHASE BLENDING **&** REACTORS. SENSOR POSITION. The sensor measures the concentration of the substance, i.e. tracer, reactant A and B, or by-product in this specified point, and the local concentration in this point as a function of time is shown in the graph.

8.5.5. Degree of reactant A conversion, batch reactor

The degree of conversion is calculated as a relation of the total decrease in the reactant A quantity to its initial quantity. The modeling is performed for the entire process duration. For the reaction type, used for modeling, the final parameter value depends on the initial quantities of reactants only.

8.5.6. Average concentration of product, batch reactor

This parameter is calculated for the entire duration of the process. For the reaction type, used for modeling, the final parameter value depends on the quantities of reactants only.

8.5.7. By-product formation rate, batch reactor

This value is estimated by integrating local by-product formation rates in the tank volume. It can sometimes be reduced by increasing the mixing intensity or changing the point of inlet of the reactant B (see **Single-phase blending & reaction - Inlet and sensor position**).

8.5.8. Average concentration of by-product, batch reactor

This value is estimated by integrating local concentrations of by-product in the tank volume. It can sometimes be reduced by increasing the mixing intensity or changing the point of inlet of the reactant B (see **Single-phase blending & reaction - Inlet and sensor position**).

8.5.9. By-product quantity, batch reactor

This value is estimated by integrating by-product formation rate with respect to the reaction time. Its final value can sometimes be reduced by increasing the mixing intensity or changing the point of inlet of the reactant B (see **Single-phase blending & reaction - Inlet and sensor position**).

8.5.10. By-product specific formation rate in a chosen point, batch reactor

Calculation of this value is based on the kinetic equation (see SINGLE-PHASE BLENDING AND REACTORS. HOMOGENEOUS CHEMICAL

REACTION input table**)** and calculated local concentrations of the reactants. VisiMix allows for estimating zones with the lowest local selectivity of the reaction.

8.5.11. Batch blending. General pattern

Use visualization of the blending process to choose optimal admixture inlet position.

8.5.12. Maximum difference in tracer concentrations.

The changes in the degree of non-uniformity of distribution of local concentration values help analyze the course of the process, especially at the beginning stage. This stage can be shortened by increasing circulation flow rate, and sometimes by choosing better inlet positions. The data on the distribution of local concentrations can be used also for choosing sensor position in the reactor (see **Single-phase blending & reaction - Inlet and sensor position**).

8.5.13. Local concentrations of tracer
Max. local concentration of tracer
Min. local concentration of tracer

These graphs illustrate degree of 'non-ideality' of the reactor from the point of mixing and distribution of tracer. Along with the maximum and the minimum concentration values, it is possible to get graphs of local concentration in any point of the tank by corresponding positioning of the sensor (see 8.5.14)

8.5.14. Tracer concentration in a chosen point, CF.

The position of the virtual sensor in the tank is specified in the input table SINGLE-PHASE BLENDING **&** REACTORS. SENSOR POSITION. The sensor measures the concentration of the tracer in this specified point, and the local concentration in this point as a function of time is shown in the graph.

8.6. Semibatch reaction

8.6.1. Average concentration of reactant A and B, semibatch reactor

In "perfect mixing" reactors, the form of the curve of average concentrations of reactants depends only on their initial concentrations in the reactor and in the inlet flow, the reaction equation and kinetic constants. In actual mixing conditions, the form of the curve of average concentrations depends also on the inlet location and the design of the mixing unit.

8.6.2. Semibatch reactor. General pattern

The program performs simultaneous visualization of both reactants' distribution in the tank. Use visualization to select optimal inlet point for reactant B.

8.6.3. Local concentrations of reactants A and B. Maximum difference in local concentrations, semi-batch reactor

The changes in the degree of non-uniformity of distribution of local concentration values help analyze the course of the process, especially at the end of the feeding period when concentration of reactant B is relatively high. For some reactions, considerable differences in local concentrations and long non-uniformity periods can lead to formation of by-products, and decrease the output. These effects can be reduced by decreasing the mixing time, and sometimes by choosing better inlet positions. The data on the distribution of local concentrations can be used also for choosing sensor position in the reactor.

These parameters are calculated for the beginning stage only, until the difference in local concentration values becomes insignificant.

8.6.4. Average concentration of product, semibatch reactor

This parameter is calculated for the entire process duration. For the reaction type used for modeling, the final value of the parameter depends on the quantities of the reactants only.

8.6.5. Degree of reactant A conversion, semibatch reactor

The degree of conversion is calculated as a relation of the total decrease in reactant A quantity to its initial value. The modeling is performed for the entire process duration. For the reaction type used for modeling, the final parameter value depends on the initial quantities of reactants only.

8.6.6. By-product specific formation rate in a chosen point, semibatch reactor

Calculation of this value is based on the kinetic equation (see SINGLE-PHASE BLENDING AND REACTORS. HOMOGENEOUS CHEMICAL REACTION input table) and calculated local concentrations of the reactants. VisiMix allows for estimating zones with the lowest local selectivity of the reaction.

8.6.7. By-product formation rate, semibatch reactor

This value is estimated by integrating local by-product formation rates over the tank volume. By-product formation rate can be reduced by decreasing the inlet flow rate of the reactant B (increasing the feeding time, see **Single-phase blending & reaction, Semibatch reactor**) and sometimes by increasing the mixing intensity, or changing the point of inlet of the reactant B (see **Single-phase blending & reaction, Inlet and sensor position**).

8.6.8. Average concentration of by-product, semibatch reactor

This value is estimated by integrating local concentrations of by-product over the tank volume. It can be reduced by decreasing the reactant B inlet flow rate (increasing the feeding time, see **Single-phase blending & reaction, Semibatch reactor**) and sometimes by increasing the mixing intensity, or changing the point of inlet of the reactant B (see **Single-phase blending & reaction, Inlet and sensor position**).

8.6.9. By-product quantity, semibatch reactor

This value is estimated by integration of by-product creation rate along the reaction time. The final value can be reduced by decreasing the reactant B inlet flow rate (increasing the feeding time, see **Single-phase blending & reaction, Semibatch reactor**) and sometimes by increasing the mixing intensity, or changing the point of inlet of the reactant B (see **Single-phase blending & reaction, Inlet and sensor position**).

8.7. Continuous flow reaction. Starting period

8.7.1. Concentration of reactant A.

This graph shows change of the reactant A concentration in the reactor during the period of process stabilzation.
Simulation of starting period is based on solution of differential equations for perfect mixing conditions. The initial conditions correspond to ‘0’ values of concentrations of the reactants A and B, reaction product and by-product in the reactor. Simulation time is defined as a function of Residence time of the flow in the reactor (see Input table Continuous flow reactor. Inlet flows).

8.7.2. Concentration of reactant B.

This graph shows change of the reactant B concentration in the reactor during the period of process stabilzation.
Simulation of starting period is based on solution of differential equations for perfect mixing conditions. The initial conditions correspond to ‘0’ values of concentrations of the reactants A and B, reaction product and by-product in the reactor. Simulation time is defined as a function of Residence time of the flow in the reactor (see Input table Continuous flow reactor. Inlet flows).

8.7.3. Concentration of product.

This graph shows change of concentration of the reaction product in the reactor during the period of process stabilization.
Simulation of starting period is based on solution of differential equations for perfect mixing conditions. The initial conditions correspond to ‘0’ values of concentrations of the reactants A and B, of

the reaction product and by-product in the reactor. Simulation time is defined as a function of Residence time of the flow in the reactor (see Input table Continuous flow reactor. Inlet flows).

8.7.4. Concentration of by-product.

This graph shows change of concentration of the reaction by-product during the period of process stabilization.
Simulation of starting period is based on solution of differential equations for perfect mixing conditions. The initial conditions correspond to ‘0’ values of concentrations of the reactants A and B, reaction product and by-product in the reactor. Simulation time is defined as a function of Residence time of the flow in the reactor (see Input table Continuous flow reactor. Inlet flows).

8.8. Continuous flow reaction. Stable state.

8.8.1. Outlet concentrations.

The data present in his table have been obtained as a result of simulation based on equations of circulation, turbulent macro-mixing and chemical reactions (see input table Chemical reaction) . Unlike the ‘perfect mixing ‘ reactors, the outlet concentrations of reactants and reaction products in a real reactor can differ significantly from the concentrations in other points of the reactor volume.

Mathematical simulation of the reactor shows dependence of the degree of non-uniformity of distribution on the reactor design, mixing intensity and reaction kinetics See also Maximum and Minimum values of local concentrations in other tables of this sub-Menu.

8.8.2. Reactant A distribution.

The data present in his table have been obtained as a result of simulation based on equations of circulation, turbulent macro-mixing and chemical reactions (see input table Chemical reaction) . Unlike the ‘perfect mixing ‘ reactors, local values of concentration of the reactant A in different points of a real reactor can differ significantly .
Mathematical simulation of the reactor shows dependence of the degree of non-uniformity of distribution on the reactor design, mixing intensity and reaction kinetics See also Maximum and Minimum values of local concentrations in other tables of this sub-Menu.

8.8.3. Reactant B distribution.

The data present in his table have been obtained as a result of simulation based on equations of circulation, turbulent macro-mixing and chemical reactions (see input table Chemical reaction) . Unlike the ‘perfect mixing ‘ reactors, local values of concentration of the reactant B in different points of a real reactor can differ significantly .
Mathematical simulation of the reactor shows dependence of the degree of non-uniformity of distribution on the reactor design, mixing intensity

and reaction kinetics.See also Maximum and Minimum values of local concentrations in other tables of this sub-Menu.

8.8.4. Reaction product.

The data present in his table have been obtained as a result of simulation based on equations of circulation, turbulent macro-mixing and chemical reactions (see input table **Chemical reaction data**) . Unlike the ‘perfect mixing ‘ reactors, local values of concentration of the reaction product different points of a real reactor can differ significantly, and outlet concentration is not always equal to the average concentration.

The presented values of the **Product yield** are based on Outlet concentration of the product and Inlet flow rates and Inlet concentrations of reactants A and B.
Mathematical simulation of the reactor takes into account dependence of the **Product yield** on degree of non-uniformity of distribution on the reactants.

8.8.5. By-product formation.

The data present in his table have been obtained as a result of simulation based on equations of circulation, turbulent macro-mixing and chemical reactions (see input table Chemical reaction) . . Unlike the ‘perfect mixing ‘ reactors, local values of concentration of the reactant B in different points of a real reactor can differ significantly, and it can cause some increase in formation of by-product.

Mathematical simulation of the reactor provides local values By-product specific formation rate as a function of mixing intensity and inlet/outlet locations. It helps to select the conditions corresponding to the minimum possible By-product formation rate for the given Reaction kinetics.

8.9. Liquid-solid mixing

8.9.1. Complete/incomplete suspension

This option is used for directly checking the conditions for complete suspension of the solid. If complete suspension is achieved, VisiMix issues a message informing you that no separation of solids is expected. If complete suspension is not achieved, VisiMix informs you of possible separation of solids.

8.9.2. Axial distribution of solid phase

This graph shows the radius average concentration of the solid phase as a function of the tank height. It does not reflect local characteristics, especially near the impeller. If the mixing in the tank is satisfactory, i.e. the non-uniformity is less than 25%, the graph gives a good description of the axial distribution of the solid phase. In case of non-satisfactory mixing, the graph can be used for general reference purposes.

8.9.3. Radial distribution of solid phase

This graph shows the height average concentration of the solid phase as a function of the tank radius. It does not reflect local characteristics, especially near the impeller. If the mixing in the tank is satisfactory, i.e. the non-uniformity is less than 25%, the graph gives a good description of the radial distribution of the solid phase. In case of non-satisfactory mixing, the graph can be used for general reference purposes.

8.9.4. Relative residence time of solid phase

This parameter is related to continuous flow processes, and is estimated as a relation of the mean residence time of the solid phase to the mean residence time of the suspension. Mean residence time of the solid phase depends on the relation of local concentration in the outlet point to the average concentration of the solid in the tank. The higher is the degree of uniformity of distribution, the smaller is the difference in the residence times for the solid and liquid phases. This difference can also be reduced by a correct choice of the outlet position.

8.9.5. Collisions of particles

This output table contains the following parameters:

Maximum energy of collisions

This parameter characterizes the energy of collisions in the zone of maximum turbulence, mainly near the impeller blades. The higher is this energy, the higher are the expected rates of crystal breaking and secondary nucleation. To decrease the energy value, try reducing the maximum local dissipation (see **Turbulence**).

Energy of collisions in the bulk volume

This parameter characterizes the average energy of collisions in the tank bulk volume. Although this energy is usually much lower than the **Maximum energy of collisions**, the number of such collisions is much higher. Therefore, they may also affect the expected rates of crystal breaking and secondary nucleation.

Frequency of collisions of maximum energy

This parameter characterizes the frequency of collisions in the zone of maximum turbulence, mainly near the impeller blades. The higher is this frequency, the higher are the expected rates of crystal breaking and secondary nucleation. It increases with the maximum local dissipation (see **Turbulence**) and the number and size of impeller blades.

Characteristic time between two strong collisions

This parameter characterizes the average duration of the period of uninterrupted crystal growth. To increase this period, try reducing the volume of the zone of maximum energy dissipation, for instance, by reducing the number of blades.
Estimation of this parameter is based on the turbulent component of the kinetic energy of particles in the most turbulized area and is related to the mean particle size.

8.9.6. Maximum and minimum local concentrations of solid phase

Comparing this parameter to **Concentration of solid phase** entered in the input table PROPERTIES OF SOLID AND LIQUID PHASES shows how homogenous is solid phase distribution in the tank.

8.9.7. Average concentration of solid phase in continuous flow

This parameter is related to continuous flow processes. The concentration of the suspension in the outlet point is assumed to be equal to the concentration in the feed flow (see **Concentration of solid phase**). The difference between the actual average concentration in the tank and the concentration in the flow depends on the degree of uniformity of axial and radial distributions and on the outlet position.

8.9.8. Maximum degree of non-uniformity (axial, radial)

This parameter characterizes the maximum deviation in local concentrations of the solid phase from the average concentration in the tank. Complete uniformity of the solid phase distribution is not always necessary. However, if actual non-uniformity is higher than 25-30%, partial settling or flotation may occur.

8.10. Liquid-liquid mixing

8.10.1. Kinetics of drop break-up

Mathematical simulation returns the "mean drop size vs. time" function. The simulation is based on calculated parameters of Turbulence, that is values of turbulent dissipation and distribution of residence time of emulsion in different zones of the tank. Increasing the number or the size of impeller blades can accelerate the process.

8.10.2. Complete/incomplete emulsification

This option is used for directly checking the conditions for complete emulsification. If complete emulsification is achieved, VisiMix issues a message informing you that no separation of emulsion is expected. If complete emulsification is not achieved, VisiMix issues a message warning of possible separation of emulsion. However, this message is only issued when you address this question for the first time.

8.10.3. Mean drop size

This parameter is calculated based on the volume density function, *φ(d)* described below in **Distribution of drops by diameter**, using the formula:

$$\int_0^{\infty} x\varphi(x)dx$$

8.10.4. Sauter mean drop size

This parameter is calculated for steady-state conditions when balance is achieved between break-up and coalescence of drops. It represents the drop size in a mono-disperse emulsion having the same specific surface area as the real emulsion.

8.10.5. Specific mass transfer area

This parameter is calculated for steady-state conditions when balance is achieved between break-up and coalescence of drops. It represents the drops/continuous phase interface per unit of media volume.

8.10.6. Distribution of drops by diameter

This option returns the volume density function *φ(d)*. The mass fraction of drops whose diameters lie in the range between d_1 and d_2 is determined as

$$\int_{d_1}^{d_2} \varphi(x)dx$$

8.10.7. Mean micromixing time inside drop

This parameter represents the characteristic duration (by order of magnitude) of uniform mixing inside the drop. It is calculated for an "average" drop, i.e. for a drop of Sauter diameter. Uniform distribution of dissolved solids inside the drop can be achieved either by drop deformation at the moment of break-up or coalescence, or by non-stationary molecular diffusion. Estimation of this parameter has been performed with respect to both mechanisms. Micromixing in turbulent flow of polydisperse emulsion is understood as a stochastic phenomenon. Therefore this parameter should be considered a characteristic value.

8.10.8. Micromixing time for disperse phase

This parameter estimates the average life of a separate drop between two consecutive acts of coalescence, i.e. without intermixing with other droplets. The duration of this period depends on the volumes of high turbulence zones.

8.10.9. Frequency of coalescence

This parameter is calculated for steady-state conditions of a balance between drops break-up and coalescence. The value of this parameter strongly depends on the presence of surfactants.

8.11. Gas dispersion and mass transfer

8.11.1. Check gas distribution

This option performs a check of gas distribution in the tank.

Suitability of the equipment to gas dispersion processes, and its efficiency depend on the possibility for the complete dispersion of gas entered under the agitator, and on the distribution of the gas bubbles in the tank volume.

Modeling of break-up and coalescence of bubbles in the bulk of flow, and calculation of gas hold-up, mass transfer area and mass transfer rate are based on the assumption that **gas bubbles are distributed in the tank cross-section and are carried down with axial circulation flow.**

Check gas distribution option in **Gas dispersion and mass transfer** submenu is selected in order to check if these conditions are satisfied.

The check is based on modeling the transport of the bubbles from the distributing device to the tank periphery with the radial component of the flow velocity, and on comparing the axial flow velocity with the flotation velocity of the bubbles.

If the main requirements mentioned above are met, VisiMix issues the message *“**Satisfactory distribution of gas in the tank is expected**”*.

If these conditions are questionable, VisiMix issues the message ***"Significant non-uniformity of gas distribution is expected"***. This message is issued once only, when you address any of the items in **Gas dispersion and mass transfer** option for the first time.

The message *“**Non-satisfactory RADIAL gas distribution by impeller is expected** ”* is issued when the calculated radial flow velocity created by the impeller is not sufficient. In these conditions, the main part of gas bubbles formed in the vicinity of the blades does not reach the peripheral, up-going branch of the axial circulation cycle, and is distributed in the central part of the tank cross-section. This reduces the axial circulation and increases the bubble size, and eventually results in the decrease of the efficiency of the mass transfer process.

The situation described above occurs usually in tanks with “small” impellers. In these cases, gas distribution can be improved by selecting an agitator with a larger **Tip diameter.**

The message *“**AXIAL circulation rate is not high enough for uniform distribution of gas**”* is issued when the calculated axial component of the flow velocity is not high enough for carrying the bubble down, and distributing the gas in zones with downward direction of the flow. If this message is not followed with the message *"**Non-satisfactory RADIAL gas distribution by impeller is expected**"*, it means that the gas is distributed only in zones with upward flow direction. In this case, a significant part of the tank volume stays “non-gassed“ and is practically excluded from the mass transfer process.

8.11.2. Gas flow number

This parameter characterizes, by order of magnitude, a ratio of volume flow rate of gas and the circulation flow rate of the media created by the impeller. It is calculated as

$$N_q = V/(ND^3),$$

where

V is volume flow rate of gas, cub. m/s
N is rotational speed of the impeller, 1/s
D is impeller tip diameter.

8.11.3. Estimated surface aeration rate

This parameter represents gas flow rate per unit of tank cross-section, and describes the entrainment of gas into the liquid caused by the turbulence on the surface. Comparison of this value to the **Superficial gas velocity** entered in GAS DISPERSION BASIC DATA input table helps evaluate the importance of the surface aeration for the tank operation (gas hold-up, mass transfer, etc.). A zero value means that no stable surface aeration occurs. However, occasional suction of gas may still take place.

8.11.4. Sauter mean bubble diameter

Calculation of bubble size is based on mathematical modeling of break-up and coalescence of gas bubbles in the bulk of flow. While real gas-liquid dispersion in a mixing tank is polydisperse, the Sauter mean diameter is the size of bubbles in a mono-disperse gas-liquid system having the same specific surface.

8.11.5. Sauter mean bubble diameter according to published empirical correlations

This value of the Sauter mean bubble diameter is calculated using the correlation proposed by P. H. Calderbank (P. H. Calderbank and M. B. Moo-Young, Trans. Inst. Chem. Engrs, 1958, V.36, No.5, p. 443). Experiments were performed in tanks with 6-blade disk turbines, tank volume – up to 100 liters, specific power 0.25-5 W/kg; superficial gas velocity – 0.005 – 0.018 m/s, viscosity of liquid 0.5 – 28 cP, interface tension 0.0217 – 0.0735 N/m.

8.11.6. Gas hold-up

This parameter represents the average value of volume fraction of gas in the gas-liquid mixture.

8.11.7. Gas hold-up according to published empirical correlations

This parameter represents **Gas hold-up** values calculated using correlations adduced in publications listed below.

Table 6. Published Gas hold-up values.

No.	Publication	Notes
1	P.H.Calderbank and M.B.Moo-Young, Trans. Inst. Chem. Engrs, 1958, v.36, no.5, p. 443.	6-blade disk turbines, tank volume – up to 100 liters, specific power 0.25-5 W/kg, superficial gas velocity – 0.005 – 0.018 m/s, viscosity 0.5 – 28 cP, surface tension 0.0217 – 0.0735 N/m.
2	C.V.Balzejak, G.P.Solomacha, Theory and Practice of Mixing in Liquid Media, Thesis of 6th All-Union Conference on Mixing, NIITECHIM, Moscow, 1982, p.86.	6-blade disk turbines, tank volume – up to 100 liters, specific power 2.5-12 W/kg., superficial gas velocity – 0.005 – 0.03 m/s, viscosity 1-22.4 cP
3	C.M.Chapman, A.W.Nienow, M.Cooke and J.C.Middleton, Chem. Eng. Res. Des., 1983, V.61, pp. 82, 167, 182. Cited after G. B. Tatterson, Fluid Mixing and Gas Dispersion in Agitated Tanks, McGraw-Hill, 1991.	Different impellers

8.11.8. Specific mass transfer area, gas-liquid

This parameter represents the mean value of gas-liquid contact surface enclosed in 1 cub. m of volume and is calculated using the calculated values of **Gas hold-up** and **Sauter mean bubble diameter.**

8.11.9. Specific mass transfer area, gas-liquid, according to published empirical correlations

This parameter represents **Specific mass transfer area** calculated using a correlation proposed by P. H. Calderbank (P. H. Calderbank and M. B. Moo-Young, Trans. Inst. Chem. Engrs, 1958, v.36, no.5, p. 443). Experiments were performed in tanks with 6-blade disk turbines, tank volume – up to 100 liters, specific power 0.25-5 W/kg.

8.11.10. Specific mass transfer coefficient, gas-liquid

This parameter, designated usually as $K_l a$, is calculated by multiplying calculated values of **Specific mass transfer area** by mass transfer coefficient:

$K_l a = K_l * a$,

where K_l is mass transfer coefficient, m/s, and a is specific mass transfer area, 1/m.

8.11.11. Specific mass transfer coefficient, gas-liquid, according to published empirical correlations

This parameter represents **Specific mass transfer coefficient** values calculated using correlations adduced in publications listed below.

Table 7. Published values for Specific mass transfer coefficient.

No	Publication	Notes
1	Klaas Van't Riet, Ind.Eng.Chem. Process Des. Dev., 1979, v.18, No.3, p.357	6-blade disk turbines, tank volume – up to 2600 liters, specific power 0.5-10 W/kg., superficial gas vel.–0.005– 0.04 m/s
2	A.D.Hickman, Proc. 6th Eur. Conf. on Mixing, Pavia, Italy, BHRA Fluid Eng., Cranfield, England, 369, 1988. Cited after G.B.Tatterson, Fluid Mixing and Gas Dispersion in Agitated Tanks, McGraw-Hill, 1991.	6-blade disk turbines, tank diameter – 2 m, H_20_2 – water system
3	M. Cooke, 1982. After G. C. Middleton, Gas –liquid dispersion and mixing, in the book Mixing in the Process Industries, Ed. N.Harnby, M.F.Edwards, A. W. Nienow, Butterworth-Heinemann, Oxford, 1992.	Air-water system
4	M.Cooke, Proc. 2th Eur. Conf. Bioreactors, BHRA Cambridge, 1988. After G. C. Middleton, Gas–liquid dispersion and mixing, in the book Mixing in the Process Industries, Ed. N. Harnby, M. F. Edwards, A.W. Nienow, Butterworth-Heinemann, Oxford, 1992.	Air-water system, combinations of one or two agitators
5	H.Wu, Chem. Eng. Sci, 1995, v. 50, p. 2801.	Tank diameter 200 mm, disk turbine
6	B.L.Efimov, G.P.Solomacha, Theory and Practice of Mixing in Liquid Media, Thesis of 2nd All-Union Conference on Mixing, NIITECHIM, Moscow, 1973, p.131.	6-blade disk turbines, tank volume up to 100 liters. Water and glycerol solutions, air and CO2. Viscosity: 1-25 cP. Surface aeration is taken into account.
7	L.N.Braginsky, V.I.Begachev and V.M.Barabash, Mixing in Liquid Media, Theor. Foundations and Calculation Methods, Chimia Publ. House, St. Petersburg (Leningrad), 1984.	Tank volume 0.01–0.25 cub. m, 6 types of impellers, 1-4 impellers on the shaft, specific power 0.02 - 30 W/kg, superficial gas velocity 0 – 0.05 m/s.

8.11.12. Media depth

Gas dispersion in tanks with **Fixed liquid volume** (see GAS DISPERSION BASIC DATA input table) causes an increase in the media level. The media depth in such tanks is calculated using the **Gas**

hold-up value**.** For tanks with **Fixed liquid level,** the **Media depth** is equal to the initial **Level of media** entered in the TANK input table**.**

8.11.13. Gas mass transfer rate, kg per hour

This parameter is used to determine rate of gas dissolution corresponding to calculated **Specific mass transfer coefficient** and to the values of gas **Mass solubility** and **Mass gas concentration in solution** which have been entered in the input table GAS SOLUBILITY**.**

8.11.14. Flooding according to published empirical correlations

Flooding is usually defined as a gas-liquid mixing regime in which gas is not fully dispersed by the impeller, and rises through the liquid in the form of big bubbles.

Flooding corresponds to a very low efficiency of mass transfer and should be avoided. Regretfully, no reliable calculation model for this phenomenon is currently available. The check performed by VisiMix is based on empirical correlations, which are applicable to disk turbine agitators only.

Sources:
A. W. Nienow, M. Konno, M. M. C. G. Warmoeskerken, and J.M. Smith, Proc. 5th Eur. Conf. on Mixing, Wurzburg, Germany, BHRA Fluid Eng., Cranfield, England, 143, 1985.
A. W. Nienow, M. Konno, W. Bujalsky, Proc. 5th Eur. Conf. on Mixing, Wurzburg, Germany, BHRA Fluid Eng., Cranfield, England, 1, 1985.
M. M. C. G. Warmoeskerken, and J. M. Smith, Fluid Mixing II, Sym. Series No. 89, I. Chem. Eng., Rugby, Warks, England, 1984.
M. M. C. G. Warmoeskerken, and J. M. Smith, Chem. Eng. Sci., v. 40, p. 2063, 1985.

All sources are cited after G. B. Tatterson, Fluid Mixing and Gas Dispersion in Agitated Tanks, McGraw-Hill, 1991.

8.12. Liquid-solid mass transfer.

8.12.1. Time of complete dissolution

The time for complete dissolution depends on particle size distribution. VisiMix uses a simplified approach, which allows to perform calculations even if the particle size distribution is not known. It regards the solid phase as consisting of a large quantity of particles of the **Average particle size**, and a small part of particles of a larger diameter, i.e. **Size of largest particles** (see input table PROPERTIES OF SOLID AND LIQUID PHASES). Therefore, VisiMix gives two estimates for the dissolution time, **Estimated dissolution time**, and **Dissolution time for largest particles**.

Estimated dissolution time is calculated based on the **Average particle size**, and it is the lower estimate of the time required for dissolving the main part of the solid particles, except for, maybe, the last 5% of the particles.

Dissolution time for largest particles represents the time required for the dissolution of the largest particles, and this is actually the time for complete dissolution of all particles.

Dissolution time for largest particles may prove to be dramatically greater than the time required for dissolving the main part of the solid phase. This is not only because of the size of the largest particles, but also because dissolution of these particles ends in a more concentrated solution.

Calculation of the dissolution time is performed only if the sum of the **Concentration of solid phase** (see PROPERTIES OF SOLID AND LIQUID PHASES input table) and **Initial concentration of dissolved solids** (see DISSOLUTION OF SOLID PARTICLES input table) is lower than the solubility of the solid phase. If the **Initial concentration of dissolved solids**, or **Concentration of solid phase** is too high, the program issues a warning that complete dissolution is impossible.

8.12.2. Concentration of dissolved solids vs. time

This graph shows an increase in the concentration of the dissolved solids in the solution in the course of the dissolution process. The calculation is performed according to a mono-disperse approximation.

8.12.3. Residual concentration of solid phase vs. time

This graph shows a decrease in solid phase concentration in the suspension as a result of the dissolution process. The calculation is performed according to a mono-disperse approximation.

8.12.4. Mass transfer coefficient vs. time (average)

Calculation of mass transfer coefficient is based on the physical model of a combined molecular and turbulent (eddy) diffusivity in the particle boundary layer. The eddy diffusivity is calculated using the Landau - Levich model of the decrease in turbulence in the boundary layer and in average turbulent dissipation rate in the mixing tank. For very small particles (the particle size is less than **microscale of turbulence),** the mass transfer coefficient depends on molecular diffusivity only, and increases in an inverse proportion to the particle size. It explains a short time increase in the mass transfer coefficient observed at the end of the dissolution process.

8.12.5. Mass transfer coefficient vs. time (maximum)

This parameter is mass transfer coefficient calculated for the zone of maximum local turbulent dissipation in the vicinity of impeller blades. See also **Mass transfer coefficient vs. time (average)**

8.12.6. Specific mass transfer coefficient vs. time (average)

This parameter is calculated as **Mass transfer coefficient (average value)** multiplied by **Specific mass transfer area.**

8.12.7. Diameter of solid particles vs. time

This graph shows the character of change in the particle size in the course of the dissolution process. The calculation is performed according to a mono-disperse approximation.

8.12.8. Specific mass transfer area vs. time

This graph shows the character of change in the specific mass transfer area in the course of the dissolution process. The calculation is performed for a mono-disperse approximation.

8.12.9. Mass transfer rate vs. time

This parameter is calculated as a product of the following four parameters:

Mass transfer coefficient (average value)
Specific mass transfer area
Volume of media
Solubility of solid phase minus **Concentration of dissolved solids**

8.13. Heat Transfer

VisiMix calculates all main parameters of the process for several operating regimes - Continuous Flow (**CF**), Batch (**BH**), Semibatch (**SB**) and Fixed temperature regime (**FT**) for the cases of liquid agent in jacket (**LA**) and condensing vaporous agent in jacket (**VA**).

8.13.1. Heat transfer area

This output table contains two parameters – the **Heat transfer area** and the **Active heat transfer area**. Both are calculated for the lower and the upper jacket sections. The **Heat transfer area** is the jacketed part of the tank wall surface, including the jacketed part of the bottom for the lower section. For a single-jacket device, the **Heat transfer area** for the upper section is zero. The **Heat transfer area** values in this table are those you entered in the TANK HEAT TRANSFER GENERAL DATA input table or those values calculated by VisiMix if no such data was entered.

Heat transfer calculations are based on the **Active heat transfer area**, which is the area of the submerged part of the **Heat transfer area.** VisiMix calculates this parameter based on the media volume in the tank. For Continuous Flow (**CF**), Batch (**BH**) and Fixed temperature regime (**FT**), the **Active heat transfer area** is constant and corresponds to the user's input of the **Volume of media** in the TANK input table. If the **Level of media** is higher than the upper edge of the jacket, the **Active heat transfer area** is calculated according to the **Level of media**, and the increase in the media level due to vortex formation is taken into account (see **Vortex parameters**). If in Semibatch (**SB**) process **Active heat transfer area** increases with the increase in the media level, VisiMix takes this into account.

8.13.2. Media temperature

This parameter represents the average temperature of the media in the tank and is the final result of heat transfer simulation. It is displayed as **Temperature vs. time** graphs**.** The simulation is performed in the range of temperatures entered by the user in the input table HEAT TRANSFER. CHEMICAL REACTION DATA AND TEMPERATURE LIMITS. If in the course of the simulation the temperature falls outside the prescribed limits, the program stops calculation and issues an appropriate message, indicating the time when this occurs. To obtain more information, a new value for the **Simulation time**, which is lower than the one indicated in the message, must be entered in the corresponding input table of HEAT TRANSFER SPECIFIC DATA for **CF**, **BH** and **SB** processes.

8.13.3. Wall temperature, media side

This parameter is calculated as the average value of temperature of the tank wall on the media side. In the case of fouling, the **Wall temperature** should be understood as the temperature of the media-side surface of the fouling layer. For **CF**, **BH** and **SB** processes, this parameter is displayed as a graph of **Temperature vs. time**, for **Fixed temperature regime** (**FT**) it is displayed as a single numerical value.

The program does not compare the **Wall temperature** with the permitted **Lower** and **Upper limits of temperature** of the media (see **Media temperature**); in cases when the media is sensitive to super-heating or super-cooling, check the **Wall temperature**.

8.13.4. Outlet temperature of liquid agent in jacket

This parameter represents the temperature of the liquid heat transfer agent at the outlet of the lower and upper jacket sections and is calculated for tanks with liquid heating/cooling agents (**LA**). For **CF**, **BH** and **SB** processes this parameter is displayed as a graph of **Temperature vs. time**, for **Fixed temperature regime** (**FT**) - as a single numerical value.

8.13.5. Inside film coefficient

This parameter represents heat-transfer coefficient on the media side. It is calculated based on a physical model of heat transfer in a turbulent flow (see **7.11.1.**). For **CF, BH** and **SB** processes the results of the calculations are displayed as graphs, and the change in the physical properties as a function of the current temperature is taken into account; for semibatch processes, the increase in the media volume is also taken into account. For **Fixed temperature regime**, a single numerical value of heat-transfer coefficient is displayed.

8.13.6. Outside film coefficient

This parameter represents heat-transfer coefficient on the jacket side. It is calculated separately for each jacket section with respect to the current temperatures of the heat transfer agent and the temperature of the wall on the jacket side. Calculation is based on well-known and tested empirical correlations (see **7.11.1.**). For **CF**, **BH** and **SB** processes, the results of calculations are displayed as graphs; for **Fixed temperature regime**, a single numerical value of heat transfer coefficient for each jacket section is displayed.

8.13.7. Overall heat transfer coefficient

This parameter is calculated for each jacket section separately. The calculation is based on the values of the **Inside film coefficient, Outside film coefficient** and the thermal resistance of the tank wall. The wall thermal resistance is based on your input of the tank **Material** and **Wall thickness** (see TANK SHELL input table). Thermal resistance of fouling is added according to your input in the TANK SHELL table**.** For **CF**, **BH** and **SB** processes, the results of calculations are displayed as graphs; for **Fixed temperature regime**, a single numerical value of heat transfer coefficient for each jacket section is displayed.

8.13.8. Heat transfer rate

This parameter represents the total heat transfer rate between the media and the heat transfer agent including both jacket sections. For **CF**, **BH** and **SB** processes, the results of calculations are displayed as graphs; for **Fixed temperature regime**, a single numerical value of heat transfer coefficient is displayed.

Positive values for the **Heat transfer rate** correspond to the heat flow from the media to the heat transfer agent (HTA); negative values for the **Heat transfer rate** correspond to the heat flow from the HTA to the media.

8.13.9. Specific reaction rate

This parameter is calculated in the course of simulation according to the values of the **Arrhenius constant** and **Activation energy** entered by the user in HEAT TRANSFER. CHEMICAL REACTION AND TEMPERATURE LIMITS input table with respect to a current media temperature. The results of calculation are displayed as a graph **Specific reaction rate vs. Time**.

8.13.10. Reaction heat

The total heat release or consumption in the tank is calculated in the course of simulation according to the user's input in HEAT TRANSFER. CHEMICAL REACTION DATA AND TEMPERATURE LIMITS input table and with respect to current values of **Concentration of reactants A and B** and **Media temperature.** The results of calculations are displayed as a graph of **Reaction heat vs. time**. Positive values correspond to heat release (exothermic reactions), negative values - to heat consumption (endothermic reactions).

8.13.11. Concentrations of reactants A and B

Calculations are based on common equations of bimolecular second-order reaction, and use the kinetic data entered in the HEAT TRANSFER. CHEMICAL REACTION DATA AND TEMPERATURE LIMITS input table**.** The results of calculations are displayed as a graph of **Concentration of reactants vs. time**.

8.13.12. Pressure head on the jacket

This parameter is calculated for tanks with liquid heating/cooling agents (**LA**). The output table contains the calculated value for the maximum possible pressure difference between the outlet and the inlet for each jacket section (the local resistance values for the inlet and outlet are not taken into account). For **CF**, **BH** and **SB** processes, **Pressure head on the jacket, max.** is calculated, which corresponds to the maximum flow resistance, i.e. to the lowest possible temperature of the heat-transfer agent in the jacket. For **FT** regime, the **Pressure head on the jacket** is calculated, for a calculated temperature of heat-transfer agent in jacket, corresponding to the **Media temperature for FT regime**.

8.13.13. Upper limit of heat transfer rate for half-pipe coil

This parameter is calculated for tanks with half-pipe coil jackets heated by condensing vaporous agent (**VA**) only. It is generally known that high condensation rates result in the high volume flow rate of the condensate and may cause "flooding" of the half-pipe coil jacket. The program estimates the maximum value of the heat transfer rate, which will not cause flooding. Calculations are based on empirical correlations verified during a long period of practical use.

The **Upper limit of heat transfer rate** for a given tank can be increased by connecting the two half-pipe coil sections in-parallel and increasing the **Number of starts** of the half-pipe coil (see HALF-PIPE COIL JACKET. SPECIFIC CHARACTERISTICS input table).

8.13.14. Mass flow rate of condensate

This parameter is calculated for tanks heated with condensing vaporous agent (**VA**). It appears in **Heat Transfer. Fixed temperature regime** submenu of the **Calculate** option only. The result of the calculations is presented as a single numerical value.
To calculate this parameter for **CF**, **BH** and **SB** processes, do the following:

1. Address **Mass flow rate of condensate. VA. FT.** in **HT FT** submenu after performing simulation;
2. Enter the lowest temperature of your process in the table MEDIA TEMPERATURE FOR FIXED TEMPERATURE REGIME accessible through **Edit input-----Properties and regime----Heat transfer----Fixed temperature regime**.
3. For **SB** simulation, enter the maximum **Volume of media** for your process in the TANK input table.

8.13.15. Liquid velocity in jacket

This parameter is calculated as the flow rate of the liquid heat transfer agent divided by the area of the jacket cross-section in the direction of the flow.

8.14. Mechanical calculations of shafts

8.14.1 Torsion shear

This output table contains the following parameters:

Allowable shear stress

Allowable shear stress is equal to 0.577 of the **Yield strength in tension** of the shaft material you entered in SHAFT MATERIAL AND IMPELLER MASS input table.

Maximum shear stress in upper shaft section

This parameter is the maximum torsional shear stress in the upper cross-section of the shaft (cross-section of the lower bearing for single- and 2-stage shafts) resulting from the maximum driving momentum due to the motor acceleration. The shaft is considered to be strong enough if the calculated stress value is lower than 0.577 of the **Yield strength in tension** of the shaft material you entered in SHAFT MATERIAL AND IMPELLER MASS input table.

Maximum shear stress in lower shaft section

This value is calculated as a torsional shear stress in the upper cross-section of the lower section of 2-stage shafts. The shaft is considered to be strong enough if the calculated stress value is lower than 0.577 of the **Yield strength in tension** of the shaft material you entered in SHAFT MATERIAL AND IMPELLER MASS input table. For single-stage shafts, this parameter is not taken into account.

8.14.2. Shaft vibration characteristics

This output table contains the following parameters:

Critical frequency

The critical frequency of vibrations is the main calculated parameter in the SHAFT VIBRATIONS CHARACTERISTICS output table. It corresponds to the first lateral natural frequency of the shaft vibrations associated with an overhung shaft. This value must not be close to the operating rotational speed of the impeller.

The shaft is considered stiff if the operating rotational speed is less than 70% of the calculated critical speed. Based on many years' practical experience, this condition is fully reliable for mixing in homogeneous liquids, as well as in liquid-liquid and liquid-solid systems. For gas-liquid systems, the impeller rotational speed must be about 60% of the critical speed. To avoid additional sources of vibrations, two more conditions are recommended:

1) The product of the shaft rotational speed and the number of blades must not equal the critical frequency of the shaft, and
2) The number of baffles in the tank must not be equal to the number of impeller blades. In tanks with an even number of baffles, it is advisable to use impellers with an odd number of blades.

Rotational frequency

Rotational frequency is the rotational speed of the shaft entered in the input table with impeller characteristics. In this output table, it is shown in rps.

Rotational to critical frequency ratio (Harmonic ratio)

This parameter is calculated as ratio of the shaft's rotational speed and its critical speed, and is included for your convenience.

APPENDIX 1. CONVERSION TABLES

Conversion of US customary and commonly used units to SI units

Parameter	**Value in US customary or commonly used units**	**Corresponding value in SI or technical metric units**
Linear sizes, Area, Volume		
Linear size	X in	25.4*X mm
	X ft	0.3048*X m
Area	X sq. ft	0.0929*X sq.m
Volume	X gal US	3.785*X liter, 0.003785*X cub. m
	X cub. ft	28.3*X liter
		0.0283*X cub. m
Specific area		
Specific area	X sq. ft/cub. ft	3.2808*X sq. m/cub. m
Mass, density		
Mass	X lbm	0.4536*X kg
	X lb. mol	0.4536*X kmol, 453.6*X mol
Density	X lbm/cub. ft	16.02*X kg/cub. m
	X lbm/gal US	119.8*X kg/cub. m
Viscosity		
Dynamic viscosity	X cP	0.001*X Pa*s
	X lbf*s/sq. ft	47.88*X Pa*s
Kinematic viscosity	X cSt	1E-6*X sq.m/s
	X sq. ft/s	0.0929*X sq. m/s
Surface tension		
Surface tension	X lbf/ft	14.59*X N/m
	X dyn/cm	0.001*X N/m
Concentration		
Concentration (mass/volume)	X lbm/1000 gal US X lbm/cub. ft	0.1198*X kg/cub. m 16.02*X kg/cub. m
Concentration (molar/volume)	X lb. mol/cub. ft	16.02*X kmol/cub. m
	X lb. mol/gal US	119.8*X kmol/cub. m
Flow rate		
Flow rate – mass	X lbm/s	0.4536*X kg/s
	X lbm/min	0.007560*X kg/s
	X lbm/h	0.000126*X kg/s, 0.4356*X kg/h

Parameter	Value in US customary or commonly used units	Corresponding value in SI or technical metric units
flow rate – volume	X cub. ft/s	0.02832*X cub. m/s
	X cub. ft/min	0.000472*X cub. m/s, 1.699*X cub.m/h
	X cub. ft/h	0.02832*X cub. m/h
	X gal US/h	0.003785*X cub. m/h
	X gal US/min	0.2271*X cub. m/h
		6.308E-5*X cub. m/s
flow rate – molar	X lb. mol/s	453.6*X mol/s
		0.4536*X kmol/s
	X lb. mol/min	7.560*X mol/s
		0.007560*X kmol/s
Velocity		
Velocity	X ft/s	0.3048*X m/s
	X in/s	0.0254*X m/s
Force		
Force	X lbf	4.448*X N
Shear stress		
shear stress	X lbf/sq. in	6895*X Pa
	X lbf/sq. ft	47.88*X Pa
Torque		
Torque	X lbf*ft	1.356*X N*m
	X lbf*in	0.113*X N*m
Energy, Power		
Energy	X lbf*ft	1.355*X J
	X B.t.u.	1.055*X kJ, 1055*X J
Power	X B.t.u./s	1055*X W
	X hp	746*X W, 0.746*X kW
Specific power, turbulent dissipation rate		
specific power (turbulent dissipation rate)	X hp/cub. ft	26.33*X kW/cub. m
	X Btu/(cub. ft*s)	37.26*X kW/cub. m
	X lbf*ft/(lbm*s)	2.989*X W/kg
	X Btu/(lbm*s)	2326 X W/kg
Specific reaction rate		
specific reaction rate	X cub. ft/(lb.mol*s)	0.0624*X l/(mol*s)
	X cub. ft(lb.mol*h)	1.734E-5*X l/(mol*s)

Parameter	**Value in US customary or commonly used units**	**Corresponding value in SI or technical metric units**
Pressure		
Pressure	X psi	0.068*X Atm
	X mm H_2O	9.806*X Pa
	X mm Hg	133.3*X Pa
	X lbf/sq. ft	47.88*X Pa
	X psi	6895*X Pa
Thermal Units		
Specific heat		
Specific heat	X Btu/(lbm*°F)	4187*X J/(kg*K)
	X cal/(kg*°C)	4.184*X J/(kg*K)
Heat conductivity		
Heat conductivity	X Btu*ft/(h*sq.ft.* °F)	1.73*X W/(m*K)
	X Btu*in/(h*sq.ft.* °F)	0.1442*X W/(m*K)
	X cal*cm/(s*sq. cm*°C)	418.4*X W/(m*K)
	X kcal*m/(h*sq. m*°C)	1.162*X W/(m*K)
Temperature		
Temperature	X °F	5/9*(X - 32) °C
	X °F	5/9*(X + 459.4) K
Energy of activation		
Energy of activation	X Btu/(lb*mol)	2.326*X J/mol
Arrhenius constant		
Arrhenius constant	X cub. ft/(lb*mol*s)	0.06243*X cub. m/(Kmol*s)
	X cub. ft/(lb*mol*h)	$1.734 \cdot 10^{-5}$*X cub. m/(Kmol*s)
Heat transfer rate		
Heat transfer rate	X Btu/(h*sq.ft)	3.155*X W/sq. m
Thermal resistance		
Thermal resistance	X °F *sq.ft*h/Btu	0.1761*X K*sq. m/W
Heat transfer coefficient		
HT coefficient	X Btu/(s* sq. ft* °F)	$2.044 \cdot 10^{4}$*X W/(sq. m*K)
	X Btu/(h* sq. ft* °F)	5.678*X W/(sq. m*K)
	X kcal/(h*sq. m*°C)	1.162*X W/(sq. m*K)

Conversion of SI units to US customary and commonly used units

Parameter	**Value in SI or Technical metric units**	**Corresponding value in US customary or commonly used units**
Linear size, area, volume		
linear size	X mm	0.03937*X in
	X m	3.2808*X ft
area	X sq.m	10.76*X sq. ft
volume	X liter	0.03531*X cub. ft, 0.2642*X gal US
	X cub. m	35.31*X cub. ft, 264.2*X gal US
Specific area		
Specific area	X sq.m/cub. m	0.3048*X sq. ft/cub. ft, 0.0254*X sq. in/cub. in
Mass, Density		
mass	X kg	2.205*X lbm
	X mol	0.002205*X lb. mol
	X kmol	2.205*X lb. mol
density	X kg/cub. m	0.06243*X lbm/cub. ft, 0.008345*X lbm/gal US
Viscosity		
dynamic viscosity	X Pa*s	1000*X cP, 0.02089*X lbf*s/sq. ft
	X cP	2.089E-5*X lbf*s/sq. ft
kinematic viscosity	X sq.m/s	1E6*X cSt, 10.76*X sq. ft/s
	X cSt	1.076E-5*X sq. ft/s
Surface tension		
surface tension	X N/m	1000*X dyn/cm, 0.0685*X lbf/ft
Concentration		
Concentration (mass/volume)	X kg/cub. m	0.06243*X lbm/cub. ft, 8.345*X lbm/1000 gal US
Concentration (molar/volume)	X kmol/cub. m (mol/liter)	0.06243*X lb. mol/cub. ft 0.008345*X lb. mol/gal US
Flow rate		
flow rate – mass	X kg/s	2.205*X lbm/s, 132.3*X lbm/min
flow rate - volume	X cub. m/s	35.31*X cub. ft/s, 2119*X cub. ft/min
	X cub. m/h	35.31*X cub. ft/h, 0.5886*X cub. ft/min, 4.403*X gal US/min

Parameter	**Value in SI or technical metric units**	**Corresponding value in US customary or commonly used units**
flow rate-molar	X mol/s	0.002205*X lb. mol/s
	X kmol/s	2.205*X lb. mol/s
Velocity		
Velocity	X m/s	3.2808*X ft/s
		39.37*X in/s
Force		
Force	X N	0.2248*X lbf
Shear stress		
shear stress	X Pa	0.000145*X lbf/sq. in
		0.02089*X lbf/sq. ft
Torque		
Torque	X N*m	0.738*X lbf*ft
		8.851*X lbf*in
Energy, Power		
Energy	X kJ	0.9478*X Btu
	X J	0.738*X lbf*ft
Power	X W	0.0009478*X Btu/s
		0.00134*X hp
	X kW	1.34*X hp
		0.9478*X Btu/s
Specific power, turbulent dissipation rate		
specific power (turbulent dissipation rate)	X kW/cub. m	0.03797*X hp/cub. ft
		0.0268*X Btu/(cub. ft*s)
	X W/kg	0.3346*X lbf.ft/(lbm*s)
		0.0004299*X Btu/(lbm*s)
Specific reaction rate		
specific reaction rate	X l/(mol*s)	16.02*X cub. ft/(lb.mol*s)
		57666*X cub. ft/(lb.mol*h)
Pressure		
Pressure	X Pa	$0.9869*10^{-6}$*X atm
	X atm	14.696* X lbf/sq. in (psi)
	X Pa	0.102*X mm H_2O
	X Pa	0.0075*X mm Hg
	X atm	1.01325*X bar
	X Pa	10*X dyn/sq. cm

Thermal Units

Parameter	**Value in SI or technical metric units**	**Corresponding value in US customary and commonly used units**
Specific heat		
specific heat	X J/(kg*K)	0.0002388*X Btu/(lbm*°F)
	X J/(kg*K)	0.239*X cal/(kg*°C)
Heat conductivity		
heat conductivity	X W/(m*K)	0.578*X Btu*ft/(h*sq.ft.* °F)
	X W/(m*K)	6.933*X Btu*in/(h*sq.ft.* °F)
	X W/(m*K)	0.00239*X cal*cm/(s*sq. cm*°C)
	X W/(m*K)	0.8604*X kcal*m/(h*sq. m*°C)
Temperature		
Temperature	X °C	9/5*X + 32 °F
	X K	9/5*X - 459.4 °F
Energy of activation		
energy of activation	X J/mol	0.4298*X Btu/(lb*mol)
Arrhenius constant		
Arrhenius constant	X cub. m/(Kmol*s)	0.01602*X cub. ft/(lb*mol*s)
	X cub. m/(Kmol*s)	57.67*10^{3}*X cub. ft/(lb*mol*h)
Heat transfer rate		
heat transfer rate	X W/sq.m	0.317*X Btu/(h*sq.ft)
Thermal resistance		
thermal resistance	X K*sq.m/W	5.678*X °F *sq.ft*h/Btu
Heat transfer coefficient		
HT coefficient	X W/(sq. m*K)	4.8924*10^{-5}*X Btu/(s* sq. ft* °F)
	X W/(sq. m*K)	0.1761*X Btu/(h* sq. ft* °F)
	X W/(sq. m*K)	0.8606*X kcal/(h*sq. m*°C)

APPENDIX 2. THERMAL RESISTANCE OF FOULING FOR VARIOUS MEDIA

Medium	**Thermal resistance, m^2*K/W**
WATER:	
Distilled water	0.00004
Sea water	0.00011
Pure service water	0.00023
Polluted service water	0.00055
River water	0.00017
Hard water	0.00025
OIL:	
Motor oil	0.00086
Lubricating oil	0.0042
Quenching oil	0.001
Transformer oil	0.00015
Vegetable oil	0.00031
Fuel oil	0.0005
Petroleum	0.0002
ACID:	
Hydrochloric acid	0.00005
Phosphoric acid	0.00005
Sulfuric acid	0.00005
Acetic acid	0.0005
SOLUTIONS & BRINES:	
Aluminate solution	0.00015
Caustic solution	0.0002
Alkaline solution	0.0004
Salt solution	0.0002...0.0005
Ammoniac brine	0.0003
MISCELLANEOUS MATERIALS:	
Scale	0.00033
Iron vitriol	0.001
Coke	0.00072
Gypsum	0.00083
Lime	0.00042
Organic heat-transfer media	0.0002
Polymer-forming liquids	0.00045
Rust	0.0005
Soot	0.01
Carbon bisulphide	0.0002
Refrigerant liquids	0.00007
Aromatic hydrocarbon	0.00018
Asphalt and residuum	0.0017

APPENDIX 3. PHYSICAL PROPERTIES OF VARIOUS MEDIA

WATER

Parameter	Temperature, ° C		
	20	40	60
Density, kg/cub m	998	992	983
Dynamic viscosity, Pa*s	0.001002	0.000651	0.000463
Heat Conductivity, W/(m*K)	0.602	0.630	0.653
Specific Heat, J/(kg*K)	4182	4179	4185
Cubic Expansion	0.000207		

HYDROCHLORIC ACID, 10% Solution

Parameter	Temperature, ° C	
	20	25
Density, kg/cub m	1055	
Dynamic viscosity, Pa*s		0.00127
Heat Conductivity, W/(m*K)	0.59	
Specific Heat, J/(kg*K)	2975	
Cubic Expansion	0.000279	

HYDROCHLORIC ACID, 20% Solution

Parameter	Temperature, ° C	
	20	25 C
Density, kg/cub m	1110	
Dynamic viscosity, Pa*s		0.00150
Heat Conductivity, W/(m*K)	0.57	
Specific Heat, J/(kg*K)	2609	
Cubic Expansion	0.000279	

HYDROCHLORIC ACID, 38% Solution

Parameter	Temperature, ° C	
	20	25
Dynamic viscosity, Pa*s		0.00217
Heat Conductivity, W/(m*K)	0.535	
Specific Heat, J/(kg*K)	2270	
Cubic Expansion	0.000478	

SULFURIC ACID , 60% Solution

Parameter	Temperature, ° C
	20
Density, kg/cub m	1498
Dynamic viscosity, Pa*s	0.00770
Heat Conductivity, W/(m*K)	0.485
Specific Heat, J/(kg*K)	2228
Cubic Expansion	0.000560

SULFURIC ACID , 75% Solution

Parameter	Temperature, ° C
	20
Density, kg/cub m	1669
Dynamic viscosity, Pa*s	0.00318
Heat Conductivity, W/(m*K)	0.329
Specific Heat, J/(kg*K)	1948
Cubic Expansion	0.000383

SODIUM HYDROXIDE, 30% Solution

Parameter	Temperature, ° C
	20
Heat Conductivity, W/(m*K)	0.58
Specific Heat, J/(kg*K)	3268
Cubic Expansion	0.000451

SODIUM HYDROXIDE, 50% Solution

Parameter	Temperature, ° C
	20
Dynamic viscosity, Pa*s	0.046
Heat Conductivity, W/(m*K)	0.565
Specific Heat, J/(kg*K)	2715
Cubic Expansion	0.000475

POTASSIUM HYDROXIDE, 10% Solution

Parameter	Temperature, ° C
	20
Dynamic viscosity, Pa*s	0.001226
Heat Conductivity, W/(m*K)	0.58
Specific Heat, J/(kg*K)	3689
Cubic Expansion	0.00031

GLYCERIN

Parameter	Temperature, ° C		
	20	100	200
Density, kg/cub m	1260	1208	1090
Dynamic viscosity, Pa*s	1.48	0.013	0.00022
Heat Conductivity, W/(m*K)	0.278	0.289	0.303
Specific Heat, J/(kg*K)	2350	2790	3340

HEAVY FUEL OIL

Parameter	Temperature, ° C		
	15	50	100
Density, kg/cub m	943.5	924.1	896.1
Dynamic viscosity, Pa*s	7.925	0,296	0.024
Heat Conductivity, W/(m*K)	0.121	0.119	0.116
Specific Heat, J/(kg*K)	1772	1895	2070

NOTE:

For all solutions, mass concentration is given.

APPENDIX 4. A LIST OF ABBREVIATIONS

BH	Batch process
CF	Continuous flow process
FT	Fixed temperature regime
HT	Heat transfer
HTA	Heat transfer agent
HTD	Heat transfer device
LA	Liquid heat transfer agent
SB	Semibatch process
VA	Vaporous heat transfer agent