

## **VISI MIX TURBULENT. HEAT TRANSFER PROCESS IN A SEMIBATCH REACTOR WITH HEAT CONSUMPTION.**

The example below was specially designed to demonstrate VisiMix capabilities in simulation of heat transfer processes based on reactor design and process characteristics. It describes a heat consuming reaction in a semibatch reactor heated with steam.

### **Problem description:**

A chemical process accompanied by heat consuming reaction is carried out in a semibatch unbaffled reactor with elliptical bottom and head, and an anchor impeller. To the media in the reactor, another reactant is added, then the mixture is heated, and the reaction starts. The required heating is provided by steam supplied into a conventional jacket. The process is run until the media in the reactor is heated to 80°C.

### **Initial data**

#### **Tank:**

Inside diameter = 2400 mm;  
Total height = 3300 mm;  
Initial level of media = 2100 mm;  
Final volume of media = 12 m<sup>3</sup>.  
Shell material is ply steel  
Wall width = 10 mm

#### **Impeller:**

Anchor, Tip diameter = 2040 mm;  
Height of blade = 2000 mm;  
Width of blade = 140 mm;  
Rotational speed = 30 RPM  
Motor power = 3000 W.

The reactor is insulated on the top and bottom, and its cylindrical part is partly jacketed. The jacket is of a conventional type, and is 1400 mm high. Jacket width is 50 mm, and the wall thickness is 10 mm. Steam under atmospheric pressure is used as a heating agent.

The media is an organic substance with the following characteristics:

Density = 1100 kg/cub. m;  
Dynamic viscosity = 0.015 Pa\*s;  
Initial temperature in the reactor = 60°C.

According to available practical data, thermal resistance of fouling in your case is similar to that for the pure service water.

The second fluid injected into the reactor has the following parameters:

Inlet flow temperature = 20°C;  
Duration of the reactant inlet = 25 minutes;  
Density of the inlet flow = 1150 kg/cub. m;  
Specific heat of inlet flow = 3100 J/(kg\*K);  
Heat consumption of the reaction is 4.1E+8 J.

**The task is to calculate the time in which the media temperature reaches 80°C.**

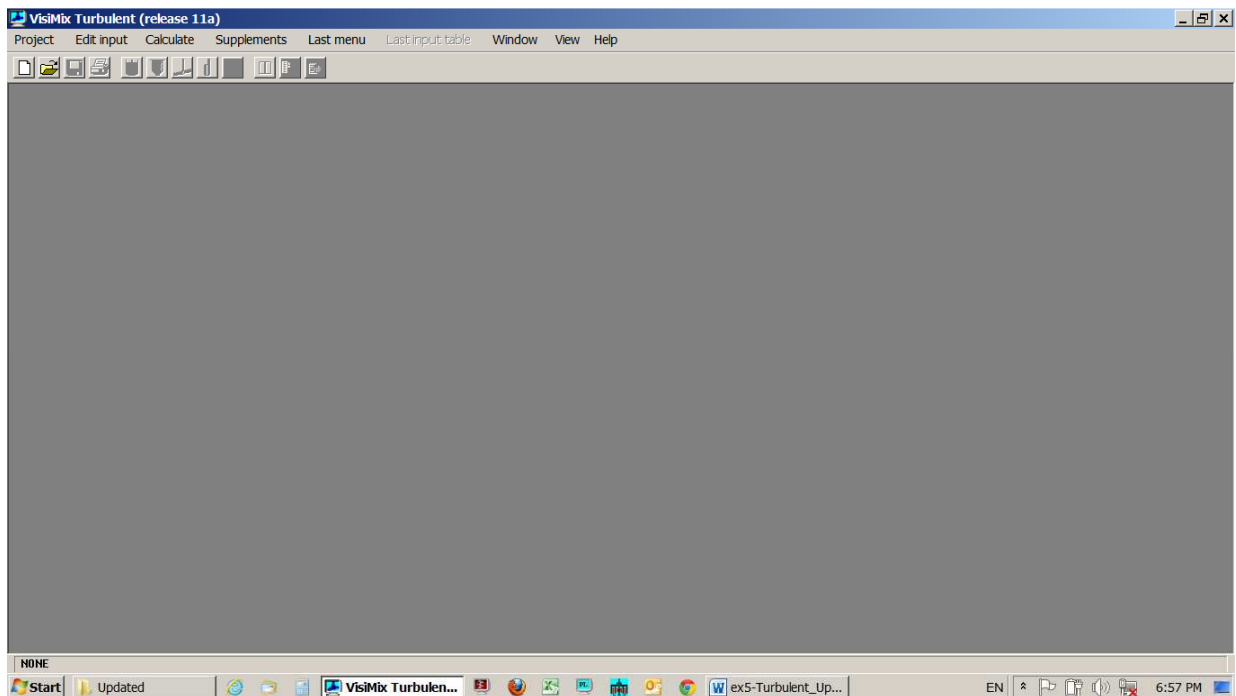
### **The Solution:**

The general sequence of operations is as follows: you must start a new project file for your case, select your tank from the graphical tanks menu, enter the initial data requested by the program, and then select the parameter you want to calculate from the **Calculate** menu. VisiMix will then request additional data required for modeling the selected parameter, and when all the requested data has been entered, you will obtain the result presented as a table or a graph.

In your case, the required parameter for calculations is **Media temperature**, in **Heat transfer. Semibatch (SB)**, **Vapor agent** in the **Calculate** menu, and the time for the temperature to reach 80°C will be determined from the output graph **Media temperature vs. time**.

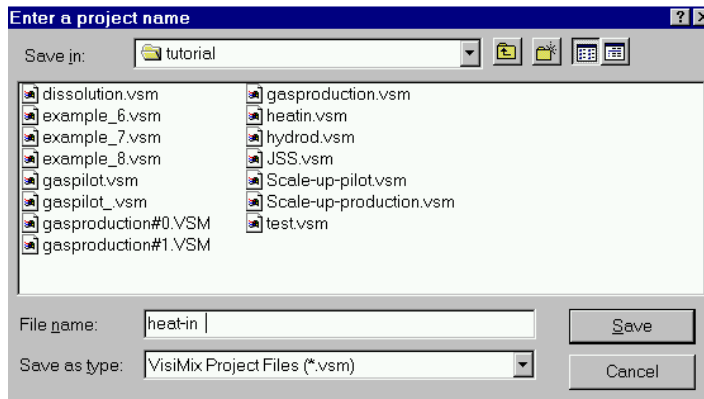
You will now follow the whole procedure step by step, from creating a new project to obtaining the desired result.

After installing **VisiMix**, the main menu appears (Figure 1). Select **Project**, then **New**, or click an appropriate quick access button in the upper screen bar.



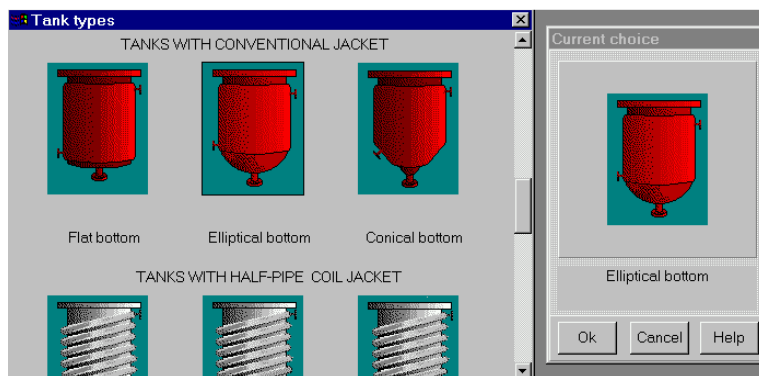
**Figure 1. VisiMix main menu.**

A dialogue table shown in Figure 2 will appear. Enter a name for the project, for example **heat-in.vsm**. You may create a special directory for your VisiMix projects, or choose an existing directory. In this example, the directory name is **tutorial**.



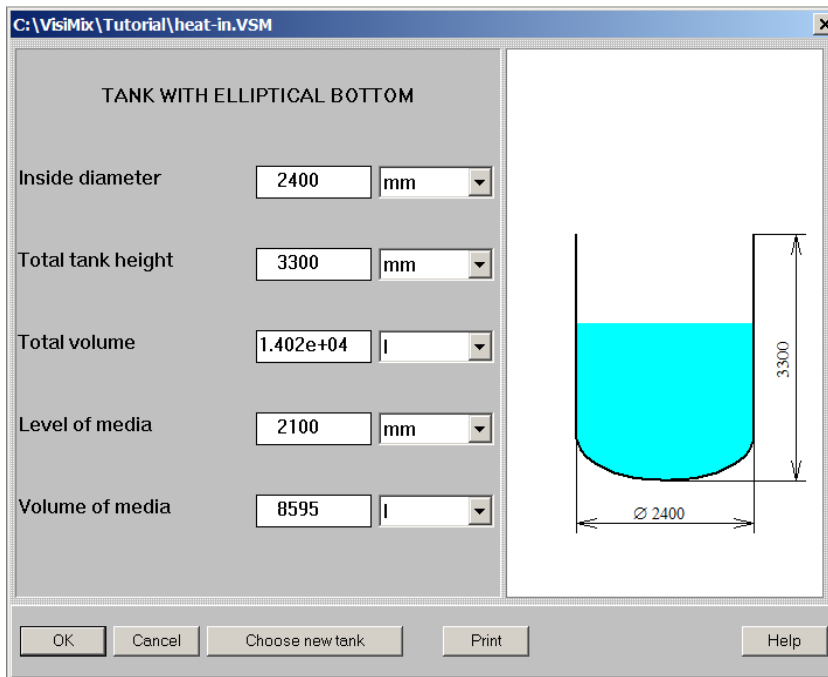
**Figure 2. Starting a new project.**

After you click **Save**, the **Tank types** menu with tanks differing by **bottom type** (flat, conical and elliptical) and **type of heat transfer device** (unjacketed tanks, tanks with conventional, half-pipe coil, and embossed/dimpled jackets) appears. To choose the required tank type, click on the appropriate tank diagram. The tank you have selected (elliptical bottom, conventional jacket for your example) will appear in the **Current choice** window on the right (Figure 3). Click **OK** to confirm your choice.



**Figure 3. VisiMix graphic tanks selection.**

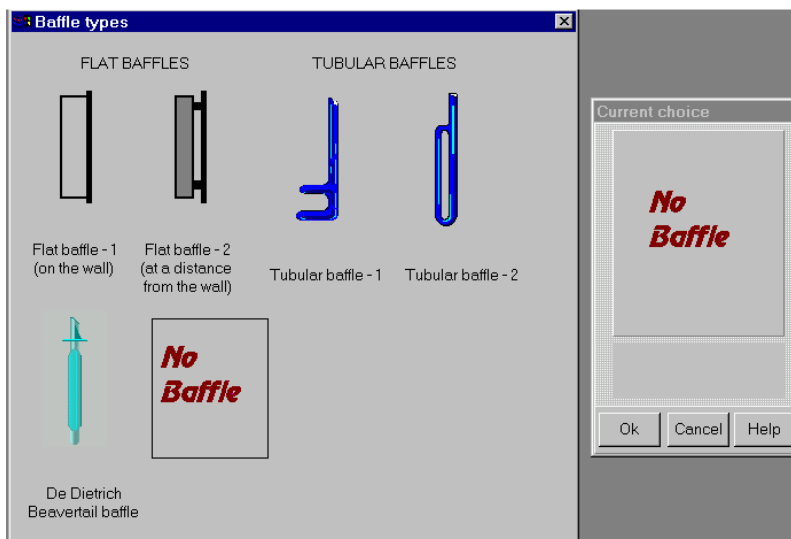
The next step is to enter the initial data for your project. You do not need to choose the initial data that must be entered. The program will request all the information it needs by invoking the appropriate input tables. At this stage, you will be asked to enter all the required tank parameters. After you confirm your tank choice, **TANK WITH ELLIPTICAL BOTTOM** input table appears. Enter **Inside diameter**, **Total tank height**, and **Level of media**, and **Total volume** and **Volume of media** will be calculated by the program and entered automatically. After the table has been completed (Figure 4), click anywhere on the field of the window, and the tank diagram on the screen will change to reflect your input. Click **OK** to confirm your input.



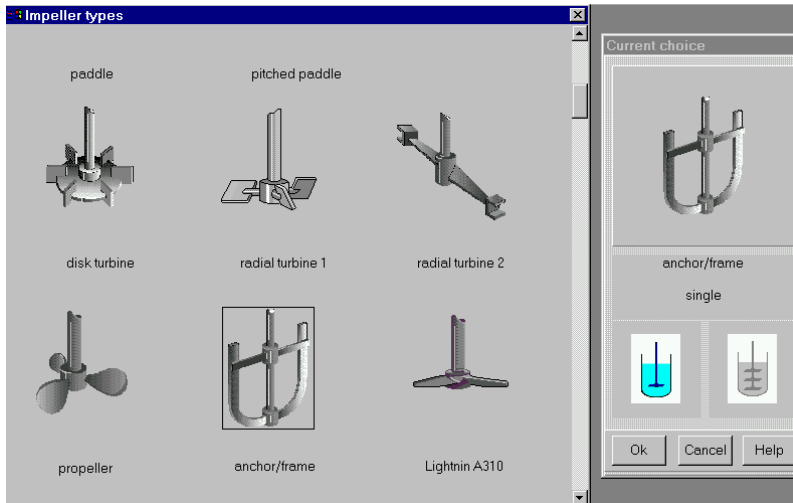
**Figure 4. Entering tank data.**

After you click **OK**, the **Baffle types** menu with different baffles (no baffle option, two types of flat baffles and two types of tubular baffles) appears. To choose the required variant, click on the appropriate baffle diagram. The one you have selected (no baffle) will appear in the **Current choice** window on the right (Figure 5). Click **OK** to confirm your choice.

**Impeller types** menu will then appear. To choose the desired impeller type, click on the appropriate diagram. The anchor impeller you have selected will appear in the **Current choice** window on the right (Figure 6). In this window, you can also select a **single**, or a **multistage** mixing system by clicking on the appropriate diagram. Your case, naturally, corresponds to a single impeller. Click **OK** to confirm your choice.

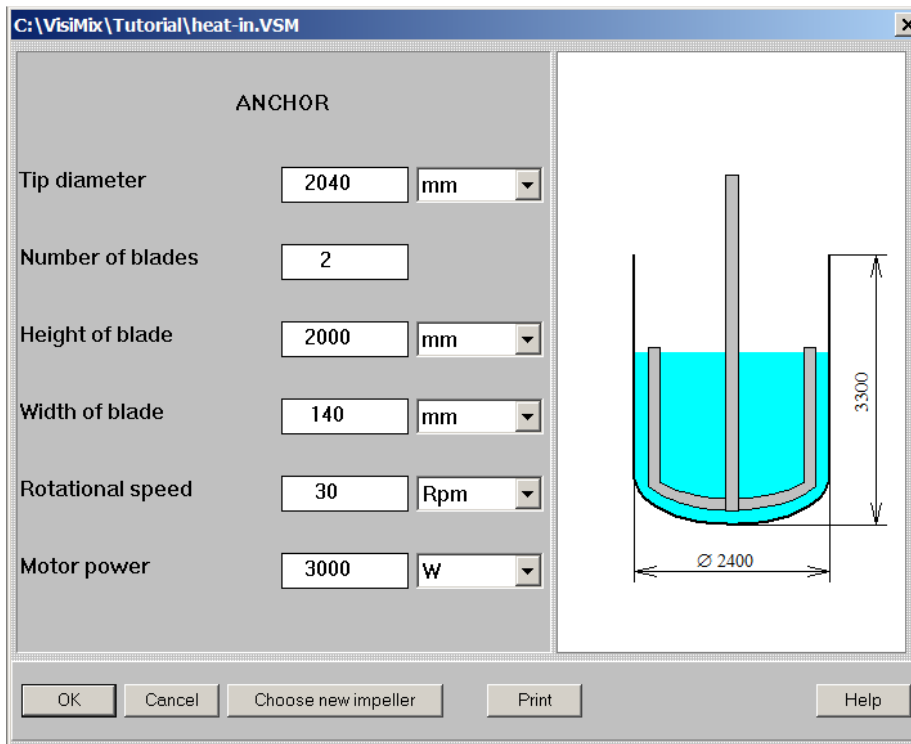


**Figure 5. VisiMix baffle selection.**



**Figure 6. VisiMix impeller selection.**

After you have selected the anchor impeller, you will be asked to fill the ANCHOR input table (Figure 7).



**Figure 7. Entering data for anchor impeller.**

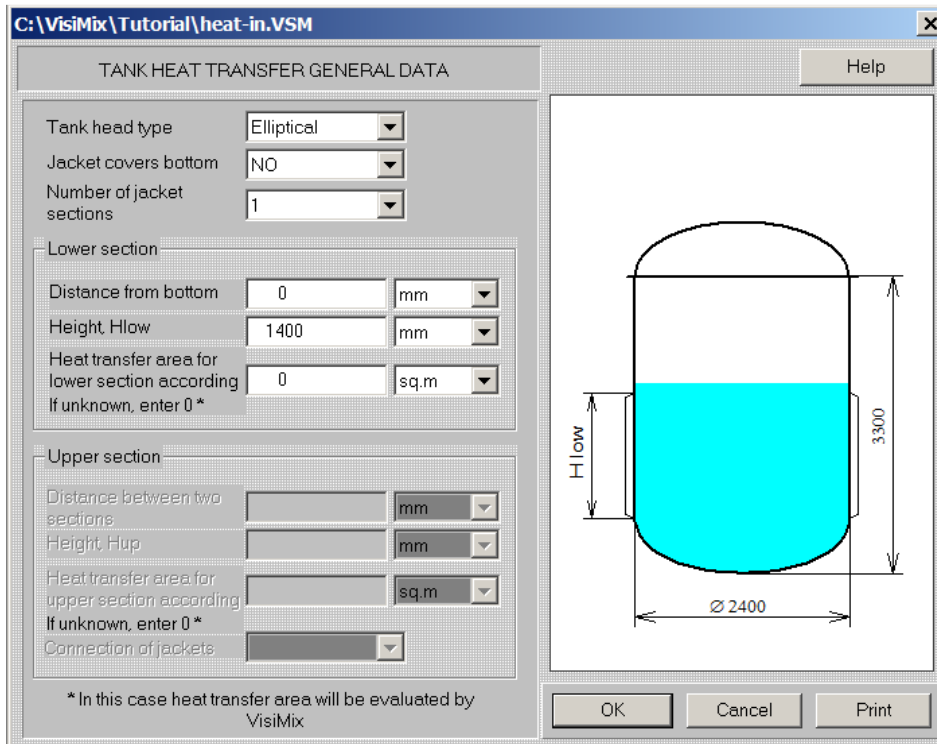
After this table has been completed, click anywhere in the field of the window, and the anchor diagram on the screen will change to reflect your input. Click **OK** to confirm your input.

You will now be asked to fill TANK HEAT TRANSFER GENERAL DATA input table with a diagram of the tank you have selected (Figure 8). Note that for a single-

sectioned jacket, only the boxes relevant to the lower jacket section will be active. The completed table includes the following data:

<b>Tank head type</b>	Elliptical
<b>Jacket covers bottom:</b>	No
<b>Number of jacket sections:</b>	1
<b>Height, Hlow (m):</b>	1400mm
<b>Heat transfer area, according to drawing (sq. m):</b>	0*

\* For **Heat transfer (HT) area**, enter the exact value if it is known to you. If not, enter “0”, and the program will calculate **HT** area according to your input.



**Figure 8. Entering general jacket characteristics.**

After this table has been completed, you will be asked to fill DENSITY AND TYPES OF MEDIA input table (Figure 9a) and AVERAGE VISCOSITY OF MEDIA (Figure 9b).

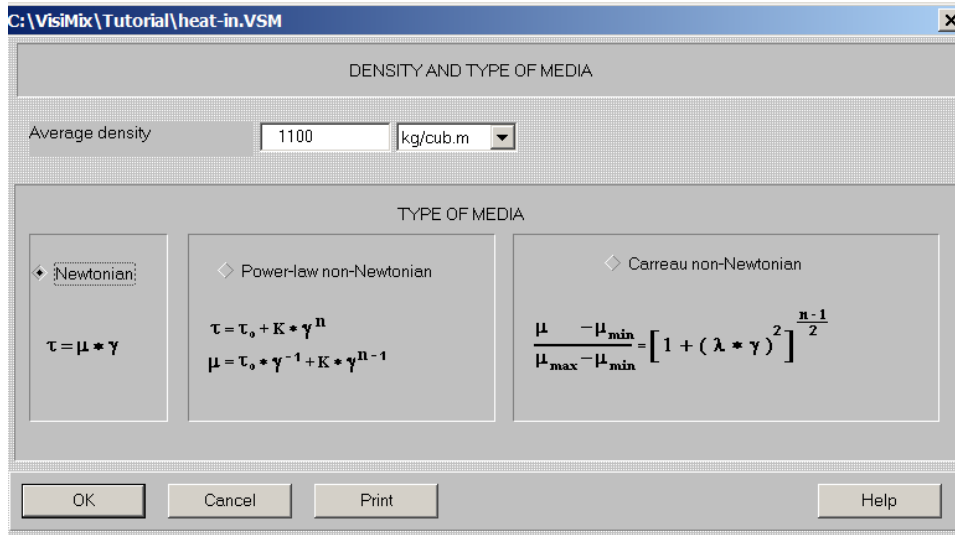


Figure 9a. Entering density and type of media.

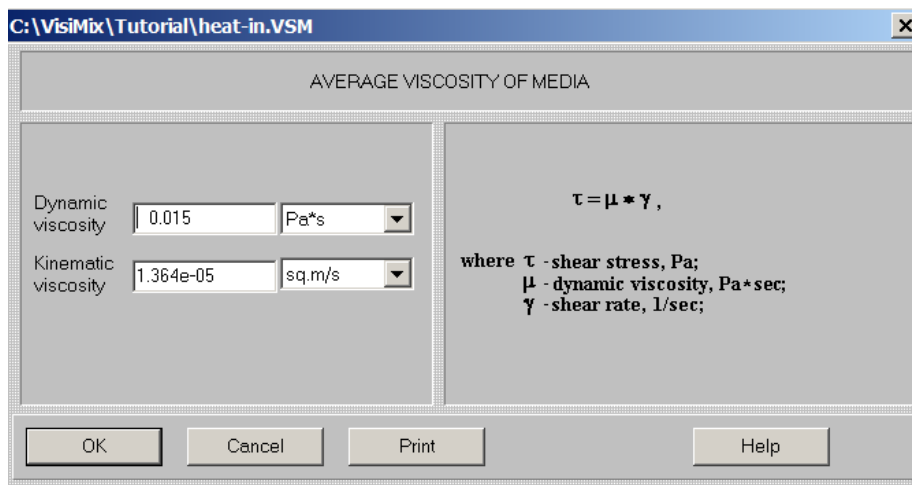


Figure 9b. Entering average viscosity of media.

Click **OK**, and a diagram of your system appears, corresponding to the data you have entered (Figure 10).

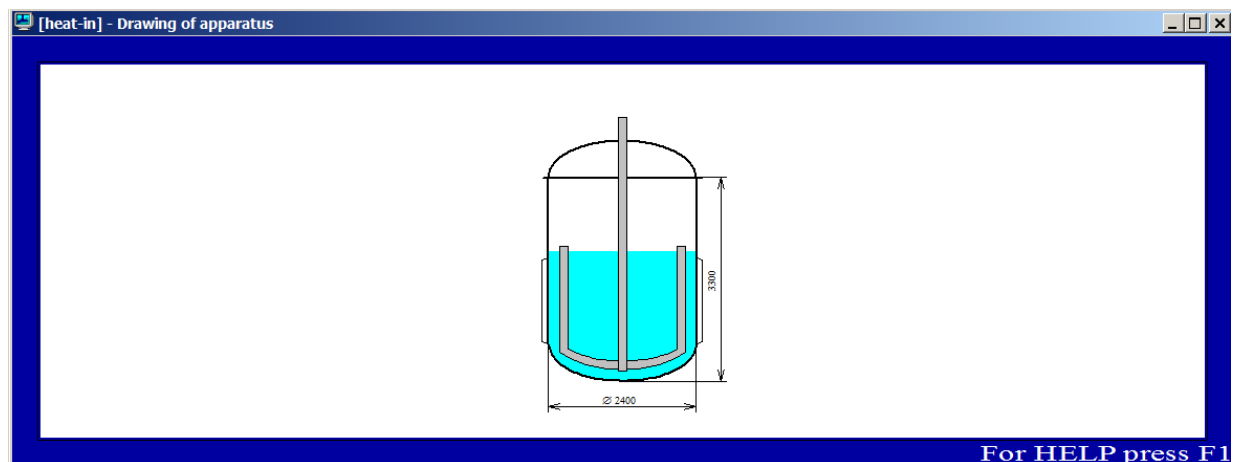


Figure 10. The diagram of your mixing system.

We recommend closing this window before proceeding to calculations. If at any stage of working on this project you will need the diagram of your apparatus, click on the appropriate quick access button in the upper screen bar.

The appearance of this diagram means that you have entered all the basic data on your equipment and media. From now on, you will be asked to enter only the data required for solving your particular problem selected in the **Calculate** option.

You can now proceed to calculations. Select **Calculate** in the main menu and click on **Heat Transfer. Semibatch (SB) and Vaporous agent (VA)**. When the submenu of output parameters appears, click on **Media temperature.SB.VA**. Since additional data is required for calculating temperature of media, VisiMix will invoke another input table: HEAT TRANSFER. CHEMICAL REACTION DATA AND TEMPERATURE LIMITS (Figure 11).

**Figure 11. Heat transfer. Chemical reaction data and regime.**

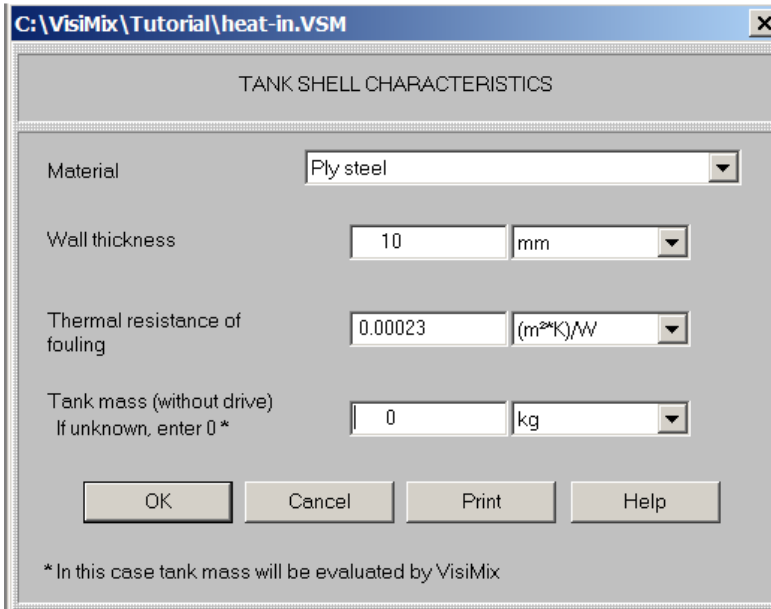
After you have completed this table, you will be asked to supply more parameters in TANK SHELL CHARACTERISTICS input table. For your example, the following parameters must be entered:

**Material:** Ply steel (*select from the list box*).  
**Wall thickness:** 10 mm  
**Thermal resistance of fouling:** 0.00023 m<sup>2</sup>\*K/W

**NOTE:** For many materials, this value can be found in *THERMAL RESISTANCE OF FOULING* table in the APPENDIX (see Help).

**Tank mass (without drive). If unknown, enter 0:**  
 The completed table is shown in Figure 12.

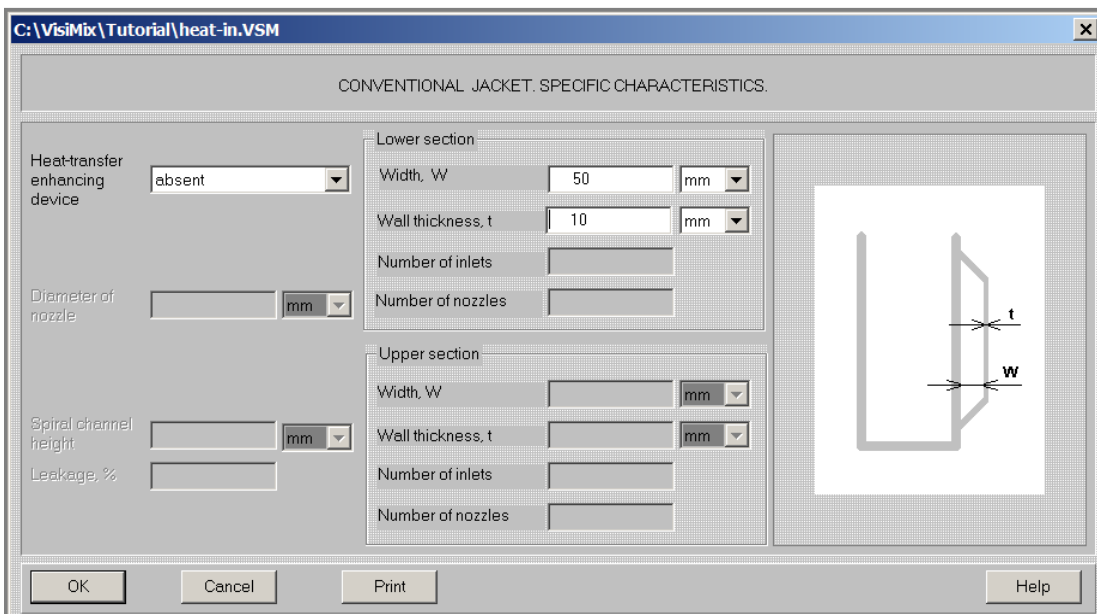




**Figure 12. Entering tank shell characteristics.**

You will now be asked to fill CONVENTIONAL JACKET. SPECIFIC CHARACTERISTICS shown in Figure 13. Input table As mentioned above, for a single-sectioned jacket, only the lower jacket boxes will be active.

The completed table is shown in Figure 13.



**Figure 13 Conventional jacket. Specific characteristics.**

You will next be asked to supply jacket data in the table called VAPOROUS AGENT IN JACKET - CONDENSATION (Figure 14). This table contains a built-in database for heating agents, which enables you to select a desired heating vaporous agent. Some basic properties of the selected heating agent appear at the bottom of the table.

**Figure 14. Vaporous agent in jacket - condensation**

After you have clicked **OK** to confirm your input, the next input table appears: HEAT TRANSFER PROPERTIES OF THE MEDIA shown in Figure 15. Upper temperature limit has been entered in accordance with your initial conditions (see above).

PARAMETER	TEMPERATURE
Average density	20 °C
Dynamic viscosity	20 °C
Specific heat	20 °C
Heat conductivity	20 °C

**Figure 15. Heat transfer properties of the media**

The last table you must complete to obtain the calculated results is SEMIBATCH PROCESS. HEAT TRANSFER SPECIFIC DATA. The completed table is shown in Figure 16.

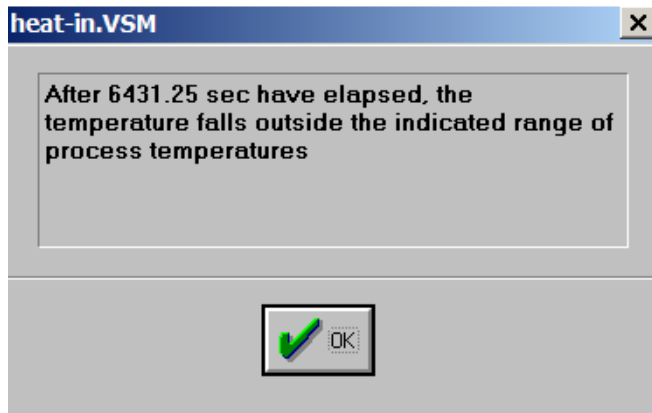
SEMIBATCH PROCESS. HEAT TRANSFER SPECIFIC DATA.

Initial temperature in the tank	60	°C	Final volume of media	1.2e+04	l
Temperature of inlet flow	20	°C	Duration of reactants inlet	25	min
Initial concentration of reactant A in the tank		mol/liter	Density of inlet flow	1150	kg/cub.m
Initial concentration of reactant B in the tank		mol/liter	Specific heat of inlet flow	3100	J/(kg*K)
Concentration of reactant A in the inlet flow		mol/liter	Heat release (consumption) for a batch	-4.1e+08	J
Concentration of reactant B in the inlet flow		mol/liter	Simulation time	125	min

Buttons: OK, Cancel, Print, Help

**Figure 16. Semibatch process. Heat transfer specific data.**

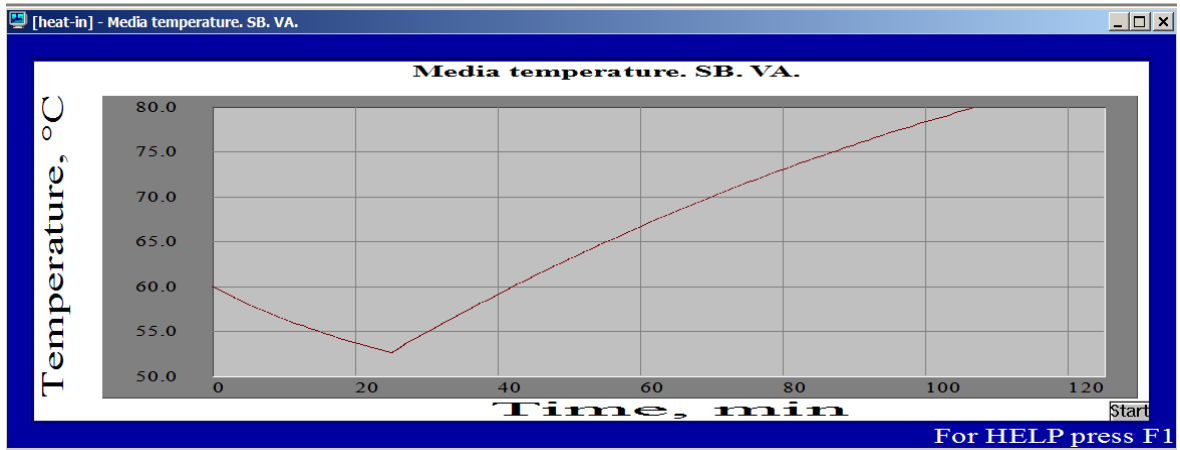
By now, you have entered all the required parameters of your equipment and process. Click **OK**, and **VisiMix** will start the calculations. In a very short time, all the required calculations will be finished, and the message shown in Figure 17 will appear. This message warns you that after 6431.25 sec (about 107 min.), the media temperature will reach the upper temperature limit (80°C in your case) that you have entered previously (see Figure 12).



**Figure 17. VisiMix warning message.**

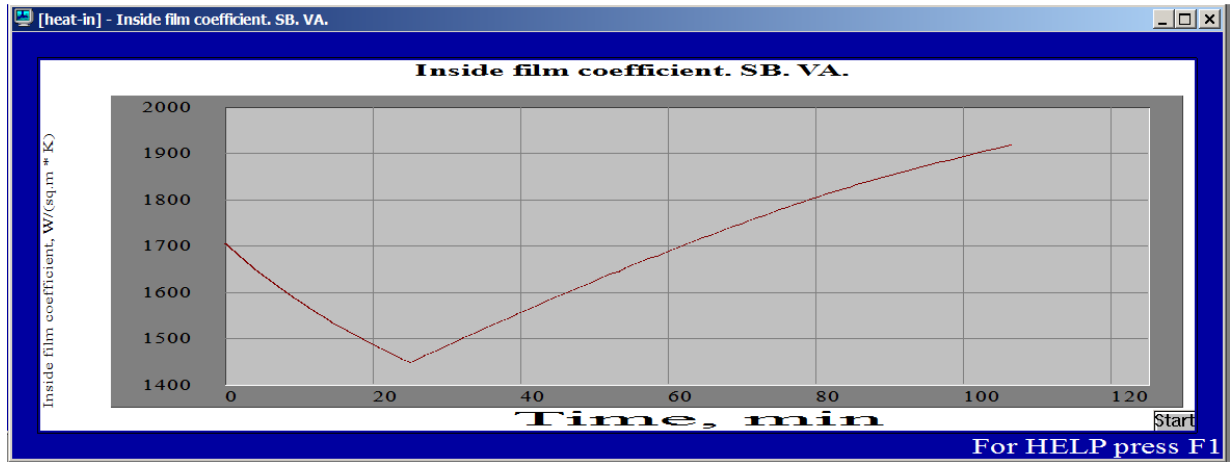
This means that in approximately 1 hour and 47 minutes, the media in the tank will be heated to 80 degrees. You have thus solved the problem and determined the heating time for your reactor.

After you click **OK**, a graph of **Media temperature. BH. VA.** appears (Figure 18). Click on the **Start** button in the lower right corner of the screen to start the simulation.



**Figure 18. Media temperature. SB. VA.**

If you are interested in other parameters in this option, just click on **Last menu** and select the required parameter. For example, **Inside film coefficient. SB. VA** is shown in Figure 19.



**Figure 19. Inside film coefficient. SB. VA.**