VISIMIX TURBULENT.

TACKLING SAFETY PROBLEMS OF STIRRED REACTORS AT THE DESIGN STAGE.

This example demonstrates usage of the VisiMix® software to provide an **Inherently Safer Design** of the process based on exothermal reaction accounting the equipment and process parameters, aiming to avoid runaway reaction that may take place when the energy generated by the reaction is greater than the energy removed from the reactor.

Problem description:

A second order irreversible reaction is carried out in a stirred batch reactor. This reaction is run according to the stoichiometry

A + B $\longrightarrow$ C

The equation for the reaction rate is:

$$r = k\, C_A\, C_B$$

where

r is reaction rate, moles of **A**/(L·sec);

k is reaction rate constant, L/(mole·sec);
C_A is concentration of reactant **A**, mole/L;
C_B is concentration of reactant **B**, mole/L.

The reaction rate constant is a function of the system temperature and is given by
$$k = k_0\, e^{-E/RT}$$

where

k_0 is Arrhenius constant, L/(mole·sec);
 E is energy of activation, kJ/mole;
 R is gas law constant, J/(mole·K);
 T is absolute temperature, K.

Kinetic reaction parameters were borrowed from the book *Safety, Health, and Loss Prevention in Chemical Processes. Problems for Undergraduate Engineering Curricula,* (The Center for Chemical Process Safety of the American Institute of Chemical Engineers) pp. 162 - 164, *Problem No. 81.*

Initial data

The reactor is a flat-bottomed tank made of stainless steel AISI 302, with a flat cover. Tank diameter is 2 m, and tank height is 2.95 m. The volume of media inside the reactor is 7.6 m³. Tank wall thickness is 8 mm, there is no fouling.

The tank has no baffles, and the impeller is a 3-stage Lightnin A310.   Tip diameter is 900 mm, distance between the stages is 500 mm, distance from bottom is 300 mm, RPM number is 120, and the motor power is 3000 W.

The reactor is insulated on top and bottom, and its cylindrical section is partly jacketed. The jacket is of a conventional type, extending from the bottom of the reactor to 0.15 m from the top.

The initial temperature inside the reactor is 20°C. Reactants **A** and **B** have the same initial concentration of 5 g-mole/L.

The actual process is performed in two stages: initial heating which starts the reaction, and subsequent cooling required for removing excessive heat. In your case, the heating is with steam at atmospheric pressure supplied into the jacket, and the cooling is with ordinary water circulated through the jacket. The average temperature of the cooling water is 20°C, and its flow rate is 40 m³/h, which corresponds to the in-jacket water velocity of about 0.035m/s.

The properties of the reacting mixture are identical to those of ordinary service water.

The maximum allowable temperature of the reactor is equal to the media vapor saturation temperature (143°C). The corresponding maximum working pressure of the reactor is 4 bar.

Heat effect of reaction is 90 kJ / mole, energy of activation is 125.5 kJ / mole and Arrhenius constant is 1E+17 liter / (mole·sec).

The task is to evaluate the suitability of your equipment to the exothermal process described above.

The Solution:

To evaluate the suitability of your equipment, you must first check a number of important general parameters, such as **Mixing power**, **Vortex parameters** and **Macromixing time**. Then you must simulate the reaction to determine the process time before the start of a runaway regime, and make sure that efficient mixing is achieved. You will then proceed to analyzing the cooling stage, and check whether the process safety is ensured.

Following the standard VisiMix procedure, you must start a new project file for your case, select your equipment, enter the initial data requested by the program, and then

select the parameter you want to calculate from the **Calculate** menu. After you have selected the parameters you want (in your case, main hydrodynamic parameters, and then parameters for simulating the exothermic reaction - heating/cooling time, concentration of reactants, etc.), the program may request additional data required for the modeling. When all the requested data has been entered, you will obtain the results: messages, tables or graphs.

It is convenient to create a separate project for each of the two process stages: heating and cooling.

After installing **VisiMix**, the main menu shown in Figure 1 appears. Let us first create a project for the first stage of the process (heating). Select **Project, New.**
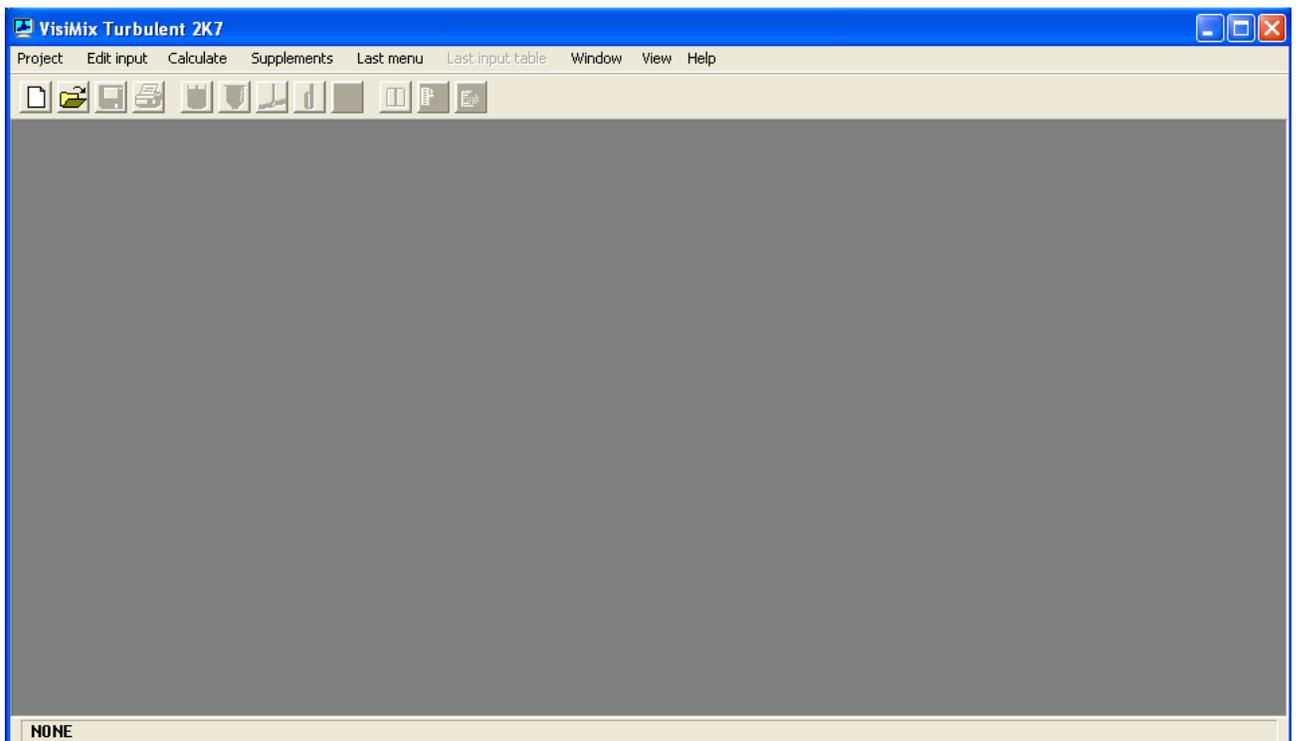
Figure 1. VisiMix main menu.

A dialogue shown in Figure 2 will appear. Enter the name for the project, for example **heat-out1.vsm**, and save it in any convenient directory. In this example, the directory name is **tutorial**.
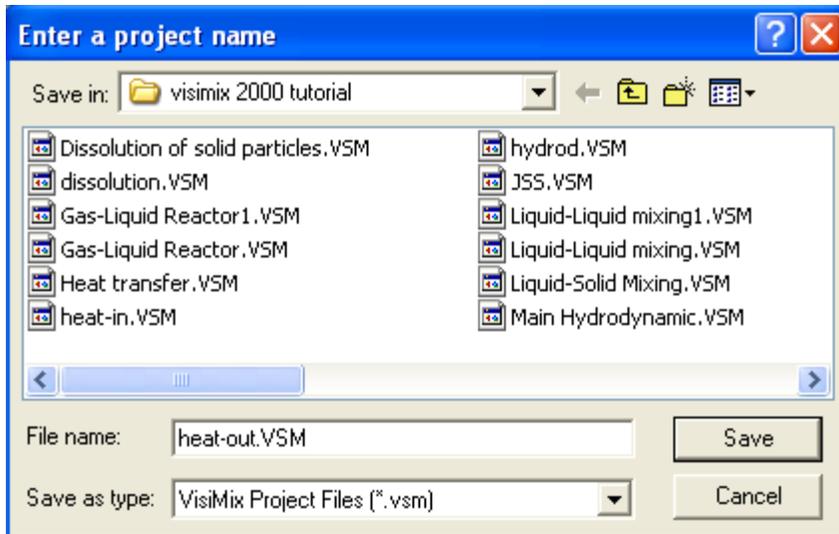
Figure 2. Starting a new project.

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. Click on the diagram of your tank (flat bottom, conventional jacket), and it will appear in the **Current choice** window on the right (Figure 3). Click **OK** to confirm your choice.

Figure 3.   VisiMix 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. VisiMix will request all the data it needs by asking you to complete 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 FLAT BOTTOM input table appears. Enter the **Inside diameter**, **Total tank height,** and **Volume of media,** and the **Total volume** and **Level of media** will be calculated by the program and entered automatically (Figure 4).
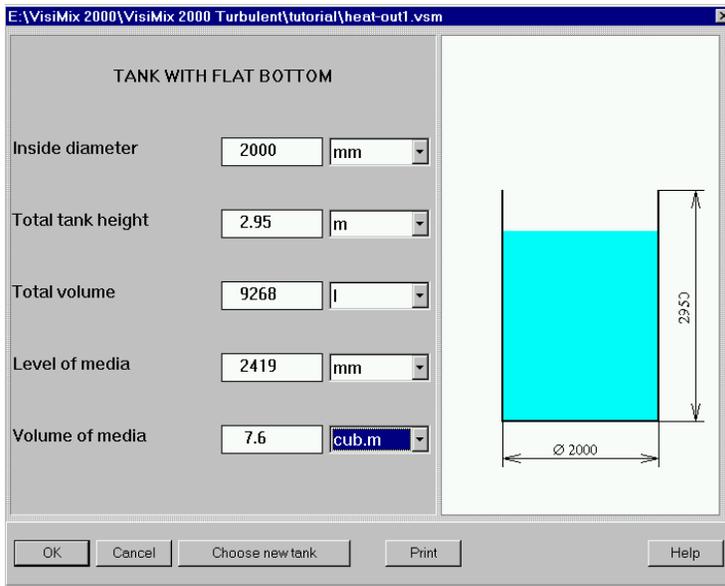
Figure 4. Entering tank data.

Click **OK** to confirm your input, and the **Baffle types** menu with different baffle options (no baffle, 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.
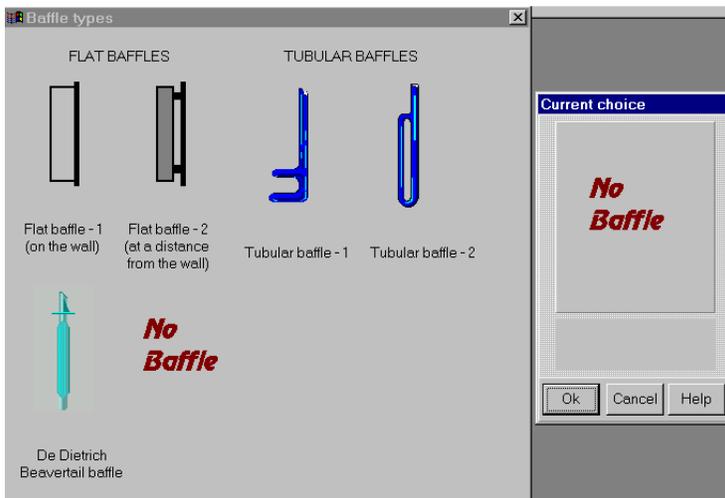

Figure 5. VisiMix baffle selection.

VisiMix **Impeller types** menu will then appear. Click on the diagram of your impeller (Lightnin A310), and it will appear in the **Current choice** window on the right (Fig. 6). Select **multistage** for you 3-stage impeller, and click **OK** to confirm your choice.

You will next be asked to supply the required parameters for your impeller. Complete the table (Figure 7), and click **OK** to confirm your input.
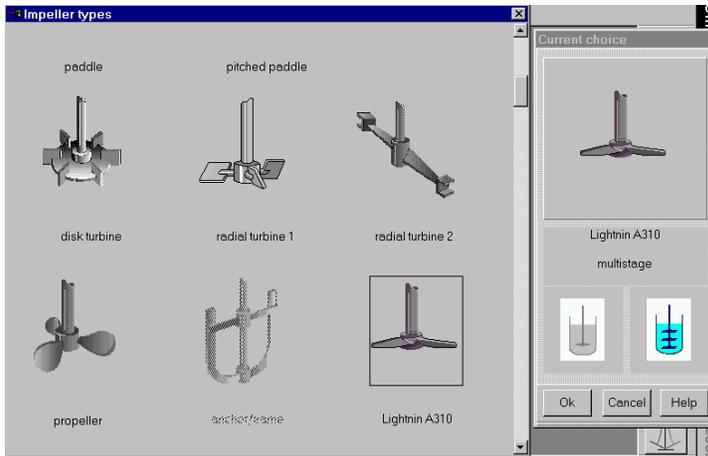
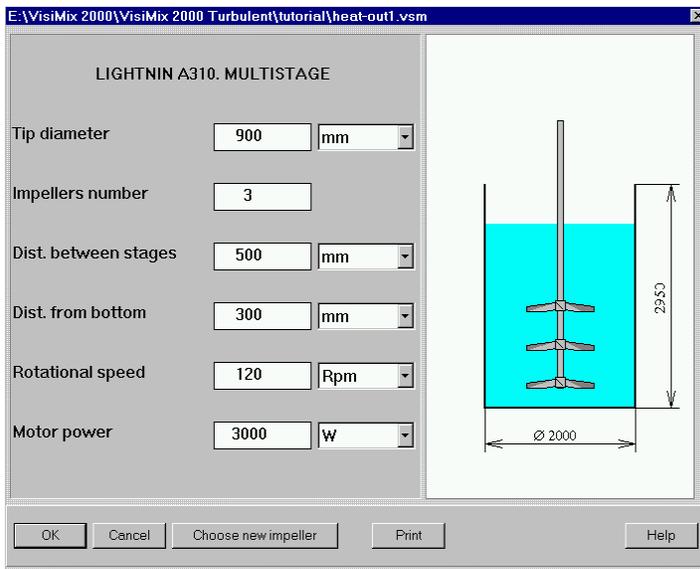*Figure 6   VisiMix impeller selection.*

Figure 7. Entering impeller data.

After this table has been completed, you will be asked to fill
TANK HEAT TRANSFER GENERAL DATA input table. Note that if the jacket has one
section, it is regarded as the **Lower section**, and the boxes related to the upper jacket
section are inactive.

Since you do not have the exact value for **Heat transfer area**, enter "0" as shown in
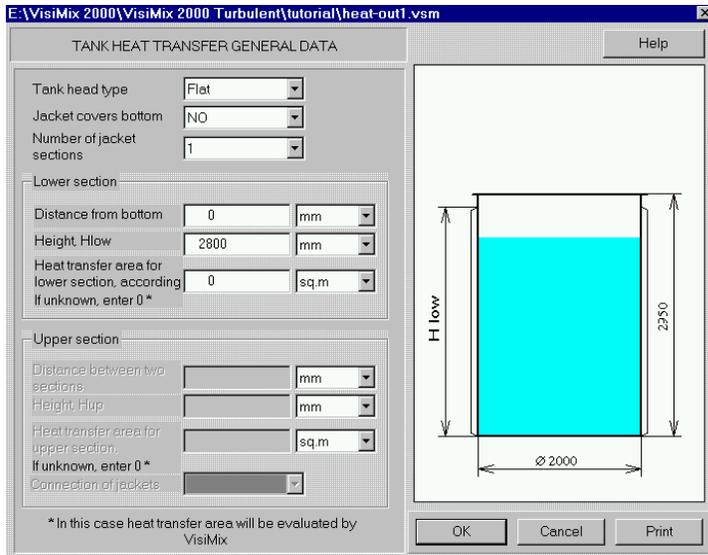Figure 8, and the program will calculate **HT** area according to your input.

Figure 8. Entering general jacket characteristics.

After this table has been completed, you will be asked to fill AVERAGE PROPERTIES OF MEDIA table (Figure 9).
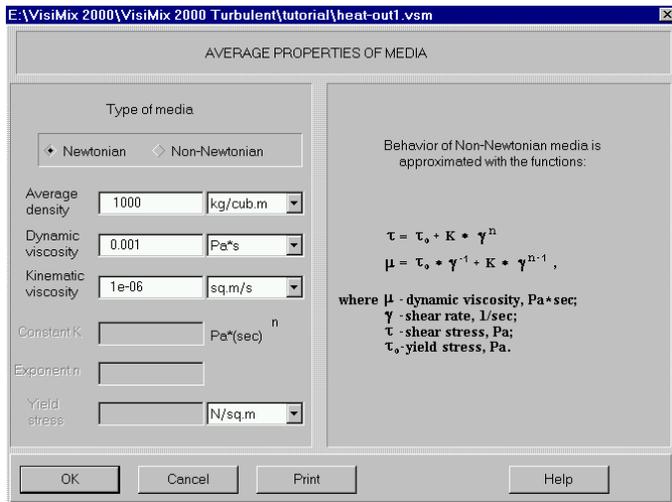
Figure 9. Entering average media properties.

In your case, the properties of the media correspond to ordinary water.

After you enter the properties of the media and click **OK,** a diagram of the selected tank appears, corresponding to the data you have entered (Figure 10).
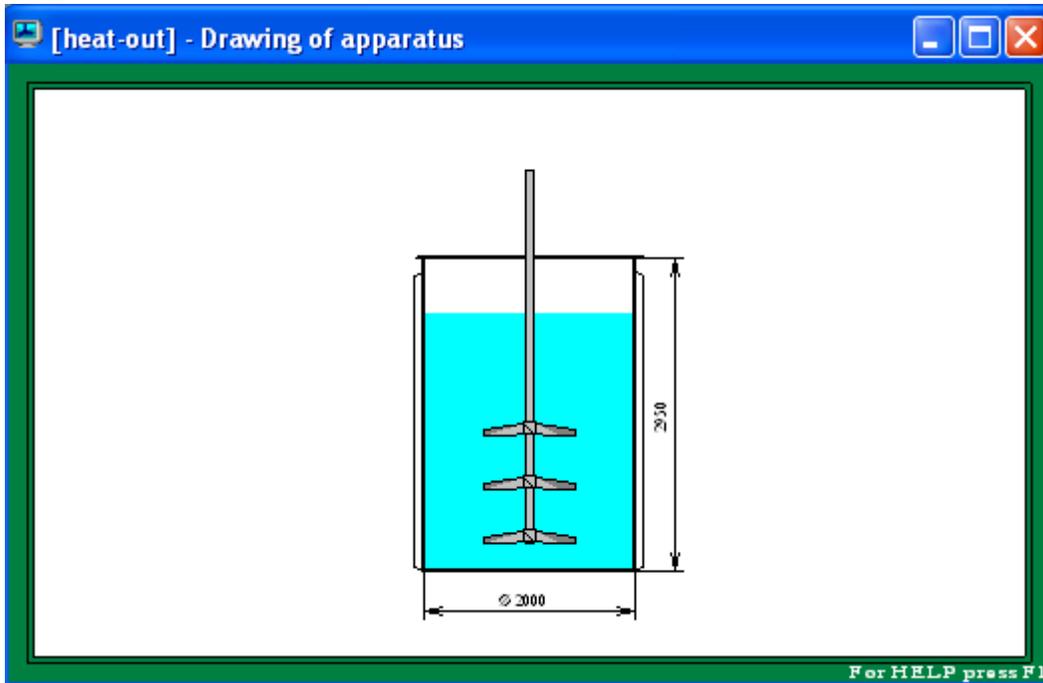
Figure 10. The diagram of the mixing system.

We recommend closing this window before proceeding to calculations.

By now, you have entered all the basic data of your equipment and properties. From now on, you will be asked to enter only the data required for solving your particular problem selected in the **Calculate** option.

Now, before examining your exothermic reaction, you should make sure that the hydrodynamic and mixing parameters of the reactor are suitable to your process. It's worth checking at least three parameters. The **Mixing power** and **Vortex** parameters are available from the **Hydrodynamics** option of the **Calculate** menu, and the **Macromixing time** - from the **Single-phase liquid mixing** option. First click on **Hydrodynamics**, **Mixing power** in order to be sure that the consumed power does not exceed the rated power of your motor (3000 W in your case, see Figure 7). The result of the calculation is shown below in Figure 11.
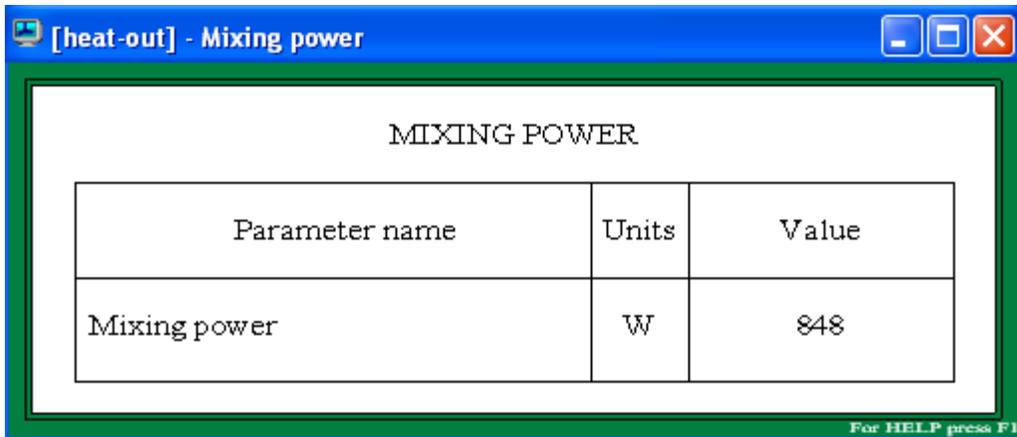
Figure 11. Mixing power.

Now you should make sure that the vortex does not reach the impeller, because if it does, the impeller efficiency will fall down dramatically. Click on **Vortex formation** in the **Hydrodynamics** submenu, and you will see that in your case the vortex does not reach the impeller (Figure 12).
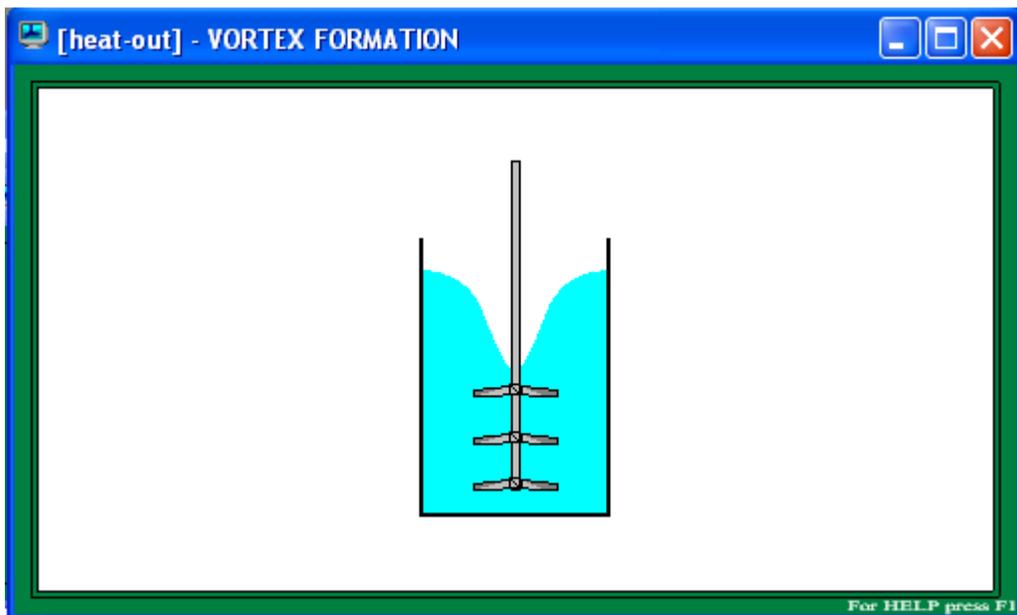

Figure 12. Vortex formation.

To obtain the third parameter needed for your general check-up, click on **Calculate, Single-phase liquid mixing** and select **Macromixing time.**

An output window with the calculated parameter will appear (Figure 13). You see that the **Macromixing time** in your reactor is about 30 sec. This result is of great practical importance. Since acceptable mixing can only be achieved if the characteristic process time considerably exceeds the macromixing time, the process time in your reactor must be not less than 300 sec (5 min).
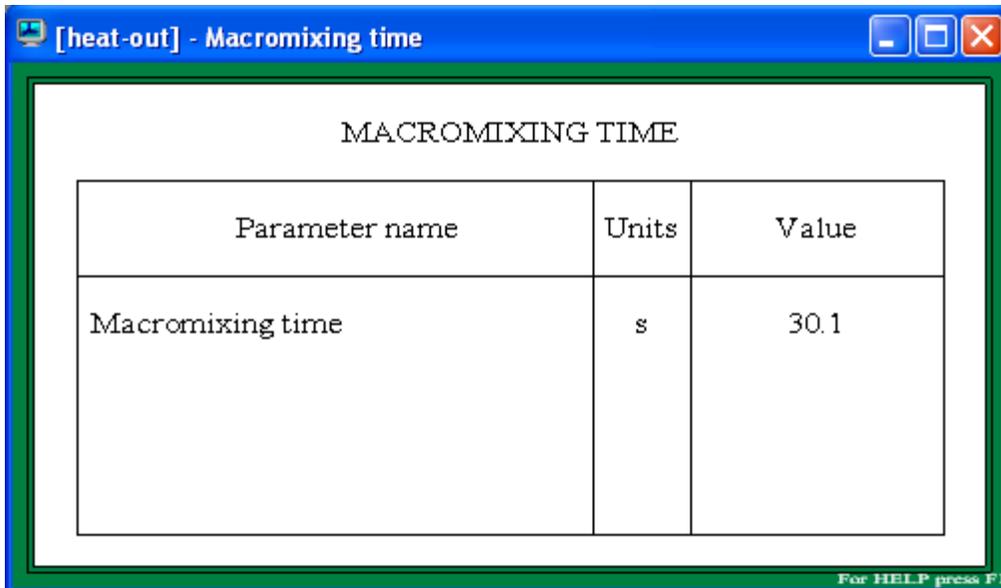
Figure 13. Macromixing time.

You can now proceed to the simulation of the exothermic process. Select **Calculate** and click on **Heat Transfer. Batch (BH) - Vaporous agent (VA).** When the corresponding submenu appears, click on **Media temperature.**

Note that while for calculations of **Hydrodynamics** and **Single-phase liquid mixing**, your input data was enough to obtain the results, the simulation of the exothermic process requires additional input parameters. You will be asked to complete HEAT TRANSFER. CHEMICAL REACTION DATA AND TEMPERATURE LIMITS input table (Fig.14). As the **Upper limit of temperature**, the maximum allowable temperature for your reactor (see above) is entered.
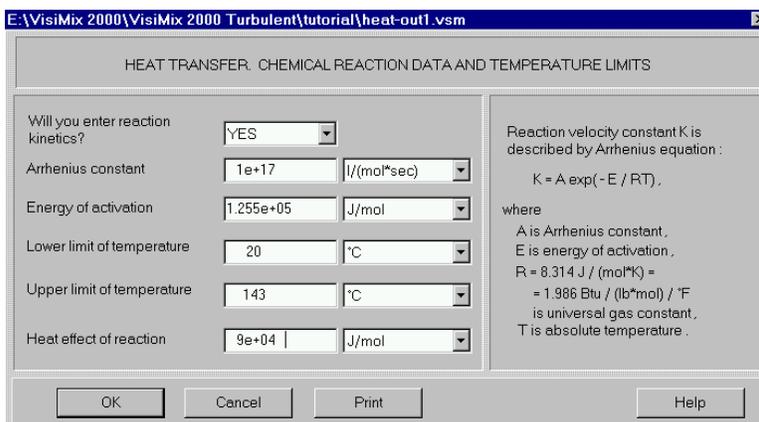
Figure 14. Heat transfer. Chemical reaction data and temperature limits.

After you have completed this table, the table TANK SHELL CHARACTERISTICS appears. The completed table is shown in Figure 15.
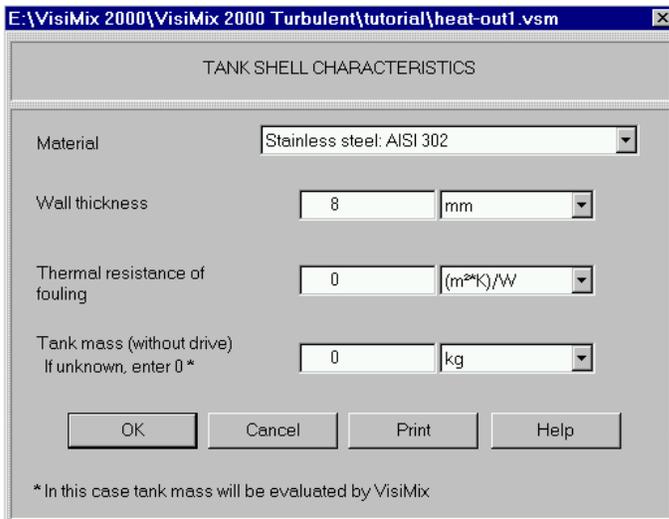

Figure 15. Entering tank shell characteristics

You will now be asked to fill CONVENTIONAL JACKET. SPECIFIC
CHARACTERISTICS input table. As mentioned earlier, for a single-sectioned jacket,
only those parameters that refer to the lower jacket section are active. The completed
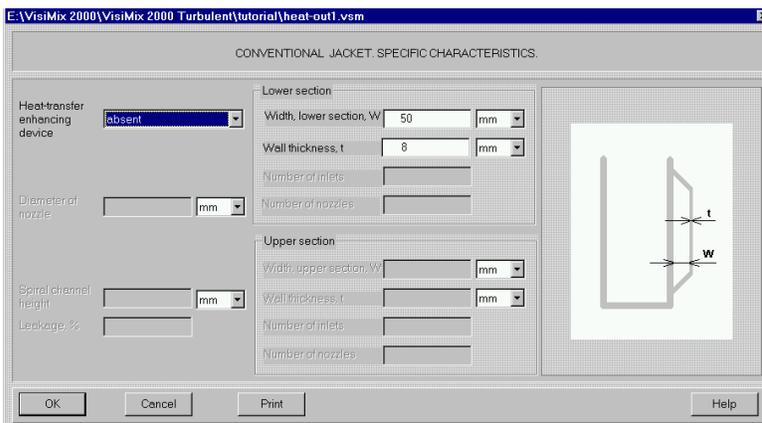table is shown in Figure 16.

Figure 16. Conventional jacket. Specific characteristics

After this table has been completed, complete the next VAPOROUS AGENT IN
JACKET - CONDENSATION, as shown in Figure 6-17. The table contains a built-in
database of heating agents. Use scrolling to select your heating agent, i.e. steam at
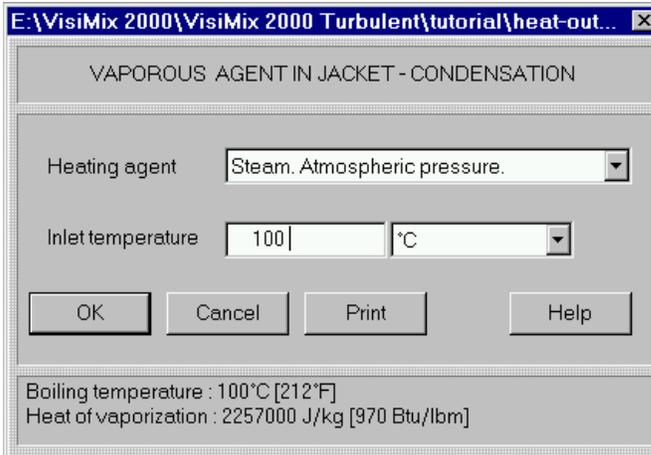atmospheric pressure, and its basic properties will appear at the bottom of the table.

Figure 17. Vaporous agent in jacket - condensation

The next input table is HEAT TRANSFER PROPERTIES OF THE MEDIA (Figure 18).
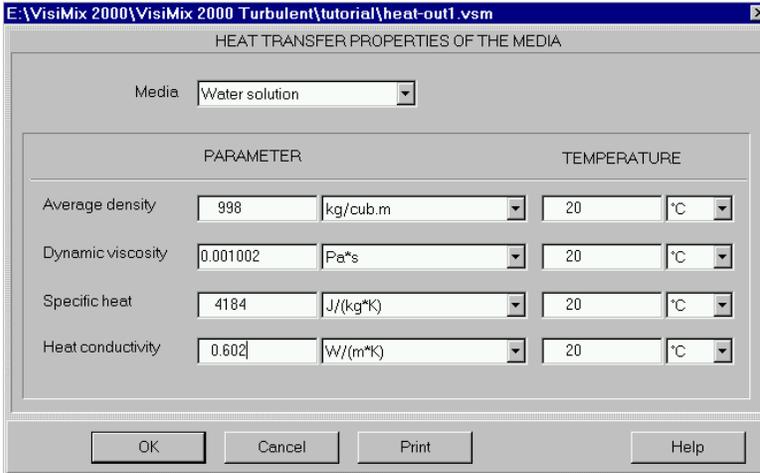

Figure 18. . Heat transfer properties of the media.

The last table you must fill is BATCH PROCESS. HEAT TRANSFER SPECIFIC DATA. The completed table is shown in Figure 19.
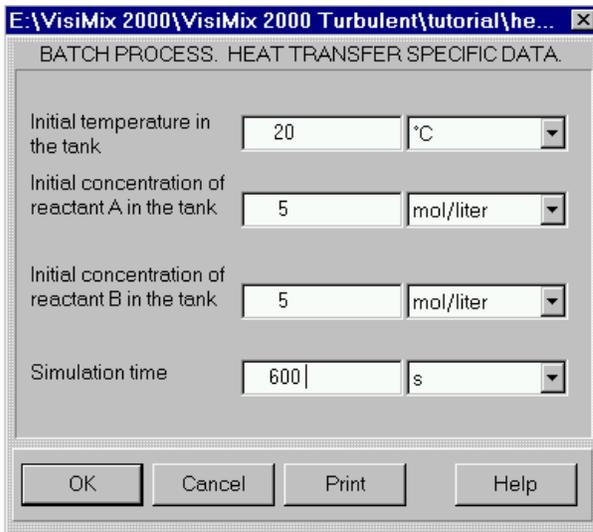

Figure 19. Batch process. Heat transfer specific data.

Now you have entered all the required parameters of your equipment and process, and VisiMix starts the calculations. In a short time, the program will issue a message shown in Figure 20, warning you that in about 8 minutes from the start the media temperature falls outside the indicated temperature range. Click **OK,** and the graph **Media temperature. BH. VA.** appears (Figure 21). Click on **Start** to start the simulation.
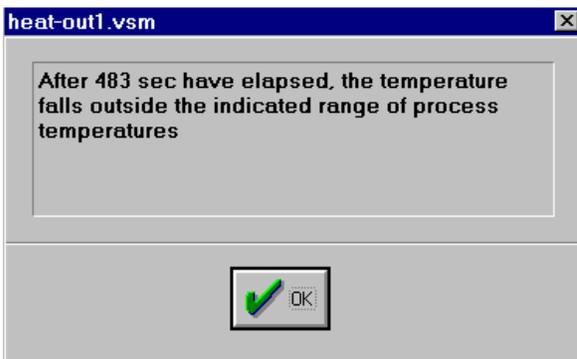

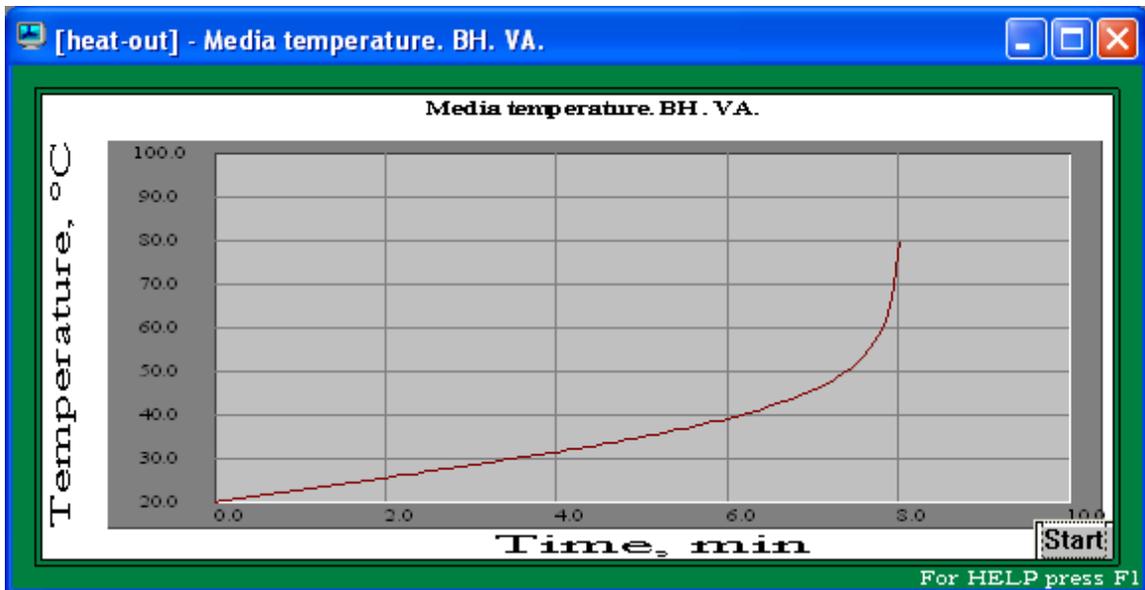*Figure 20. The message warning of the temperature exceeding the prescribed limit.*

Figure 21. Media temperature. BH. VA.

The graph shows that your process approaches a runaway regime even earlier, approximately 6 minutes from the start. Let us now check what's going on with the reaction. Click on **Last menu**, **Concentration of reactant A. BH. VA**. The appropriate output window is shown in Figure 22.
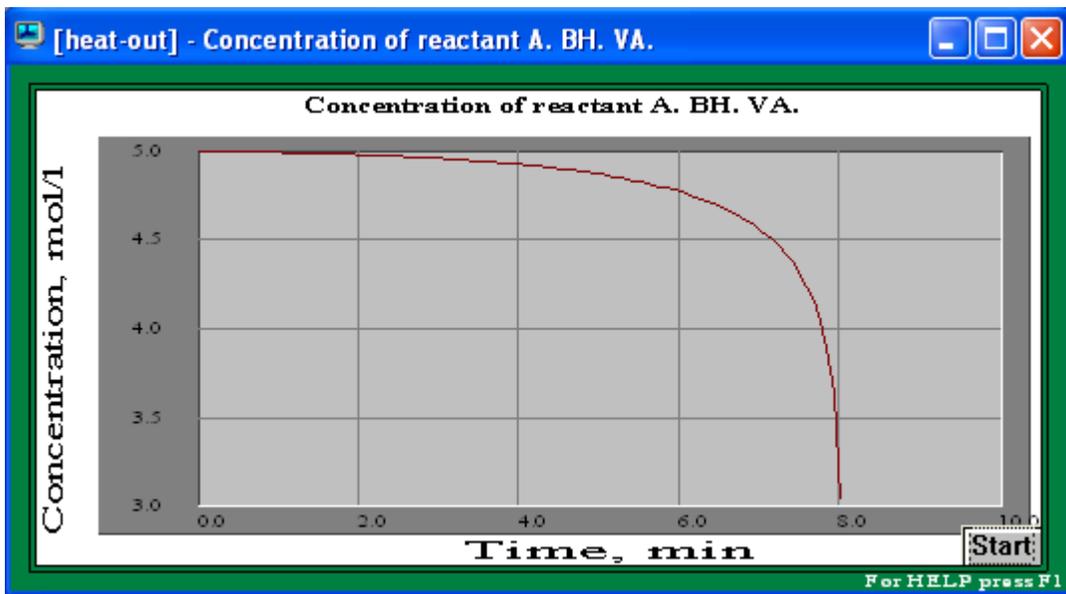

Figure 22. Concentration of reactant A. BH. VA.

As seen from Figs 21 and 22, the runaway regime is approached almost at the end of the reaction, when the reactant concentration is dramatically falling down, in about 6 minutes from the start of the process. This time is more than twenty times higher than the **Macromixing time** (30.4 sec, Figure 13). This corresponds to the basic requirement for the efficient mixing, and your reactor, therefore, may be considered as well stirred.

Now let's consider the second (cooling) stage of the process. You should start the cooling before your process approaches the runaway regime, i.e. about 6 minutes from the start of the process. At this moment the steam supply stops, the cooling water fills the jacket, and the second (cooling) stage starts. The results of the heating stage will thus serve as the initial data for the cooling stage of the simulation. Therefore, you should note the values of temperature and reactant concentration in Figures 21 and 22 corresponding to 6 minutes from the start of the process. The desired values are 40°C and 4.75 mole/liter (for both reactants).

Now you should create a project for the cooling stage of your process. Select **Window, Close All** to close all open windows. Save the current project, then use **Save as** or **Clone** option to save the current project as, for instance, **heat-out2.vsm**. You should now enter the initial data for the cooling stage by modifying some of the initial data that has been previously entered. Click on **Edit input, Properties & Regime, Heat Transfer.** First, select **Heating / cooling liquid agent** and enter the data for your cooling agent in accordance with the initial data, as shown in Figure 23.

Then select **Batch** in the same input menu. Enter the data corresponding to 6 minutes from the start of the heating stage as shown in Figure 24.
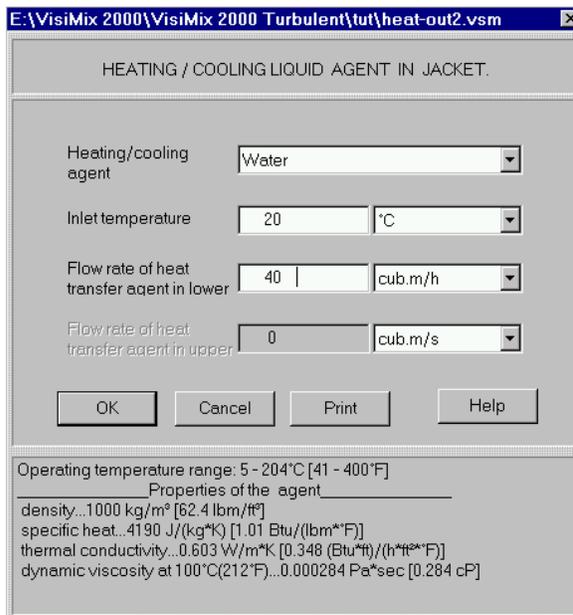

Figure 23. Cooling liquid agent in jacket (cooling stage).

To perform calculations for the cooling stage, select **Heat Transfer. Batch**, **Liquid agent (LA)** in **Calculate** and click on **Media temperature. BH. LA**, then **Concentration of reactant A. BH. LA**.
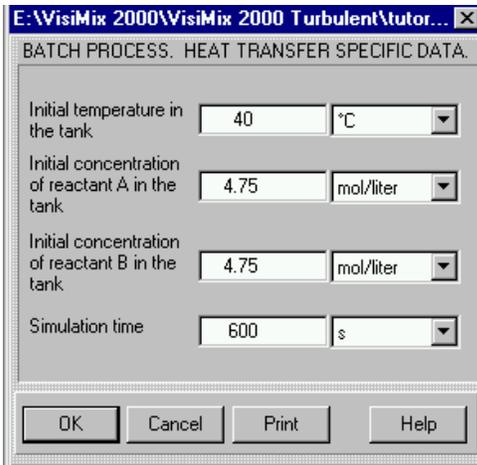
Figure 24. Batch process. Heat transfer specific data for the cooling stage.

The results of calculations are shown in Figs 25 and 26. They show that we have started the cooling early enough to prevent the process from reaching the upper temperature limit (143°C) and, consequently, the reactor maximum working pressure of 4 bar. Comparing the figures, you see that heat release stopped for the only reason that both reactants in the reactor had ended (about 2 min. from the start of the cooling). The total duration of the process is about 8 min., and only then the temperature in the reactor decreases.
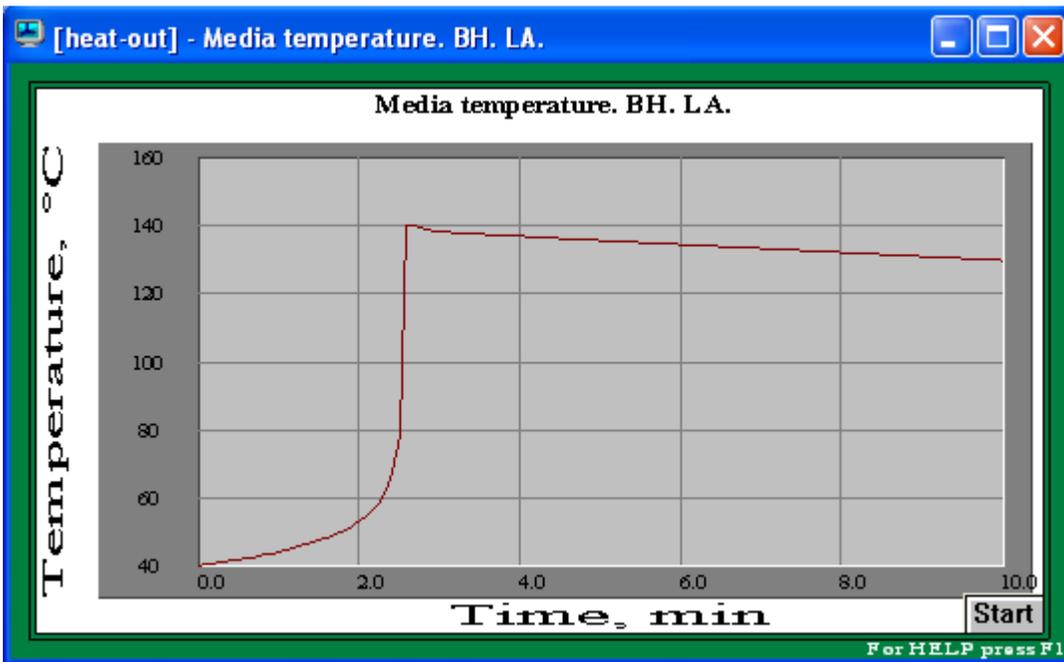

Figure 25. Media temperature. BH. LA. The heating stage is 6 minutes.
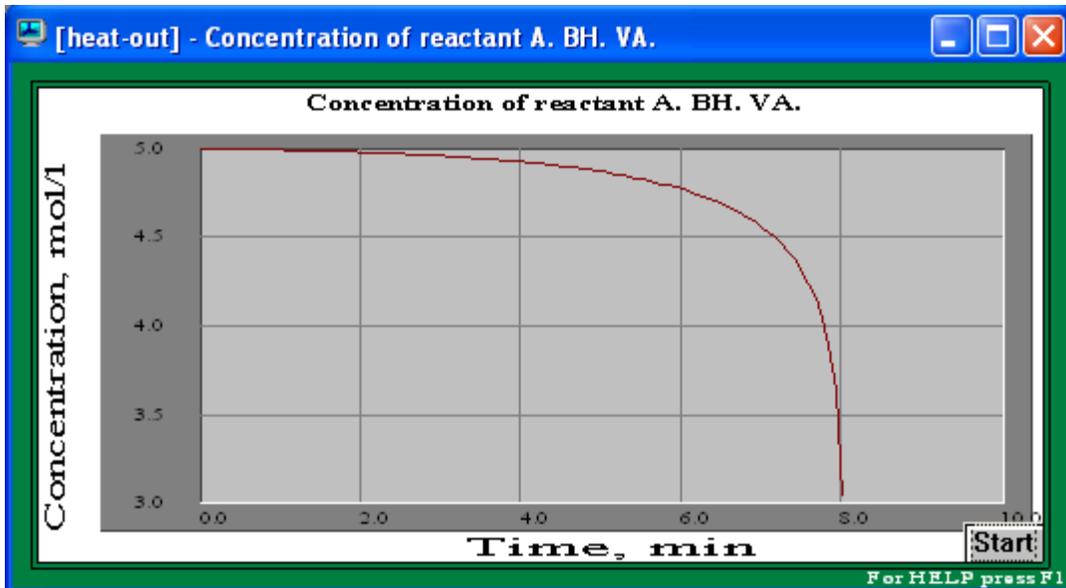
Figure 26. Concentration of reactant A. BH. LA. The heating stage is 6 minutes.

We have thus checked that if cooling starts 6 minutes from the start of the reaction, runaway regime is prevented, and the reaction is completed. However, switching from steam to cold water is not instant and in real life it may take about 1 minute. Therefore, for greater safety we should try switching to cooling a little earlier, let us say 5 minutes after the start of the process. This scenario will obviously be better from the safety viewpoint. However, we must make sure that the heating stage will be sufficient for completing the reaction.

To perform the simulation for this scenario, you must enter the appropriate values for temperature and concentration from the heating stage as initial data for the cooling stage. Return to **heat-out1.vsm**, Figures 21 and 22, and note the values corresponding to 5 minutes from the start of the process. The desired values are 35°C and 4.85 mole/liter, respectively. Now go again to the input table BATCH PROCESS. HEAT TRANSFER SPECIFIC DATA, and enter these values as shown in Figure 27.

Figure 27. Batch process. Heat transfer specific data for cooling stage. The heating stage is 5 min.

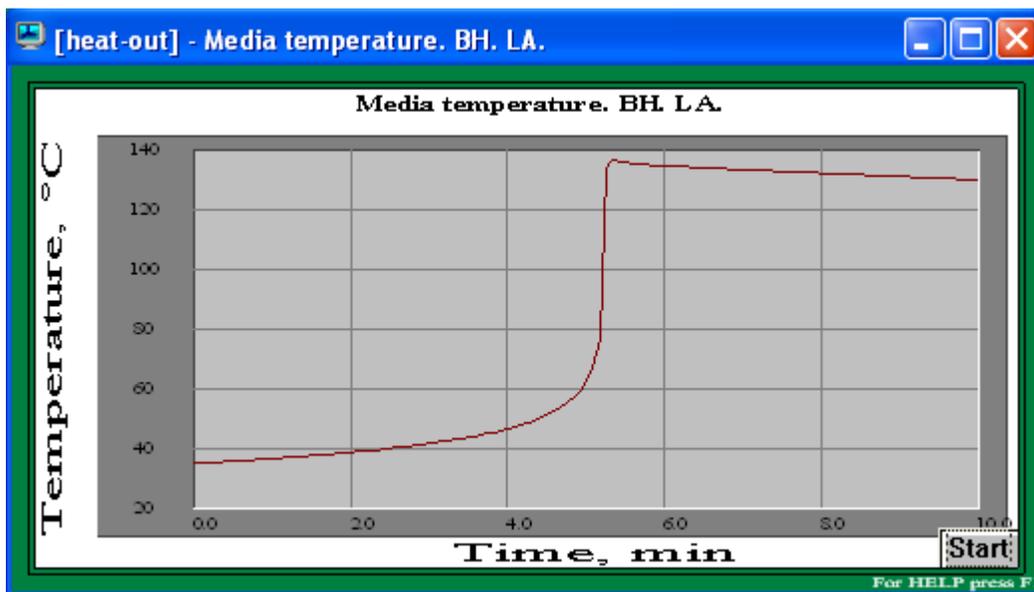The corresponding graphs are shown in Figs 28 and 29.

Figure 28. Media temperature. BH. LA. The heating stage is 5 min.
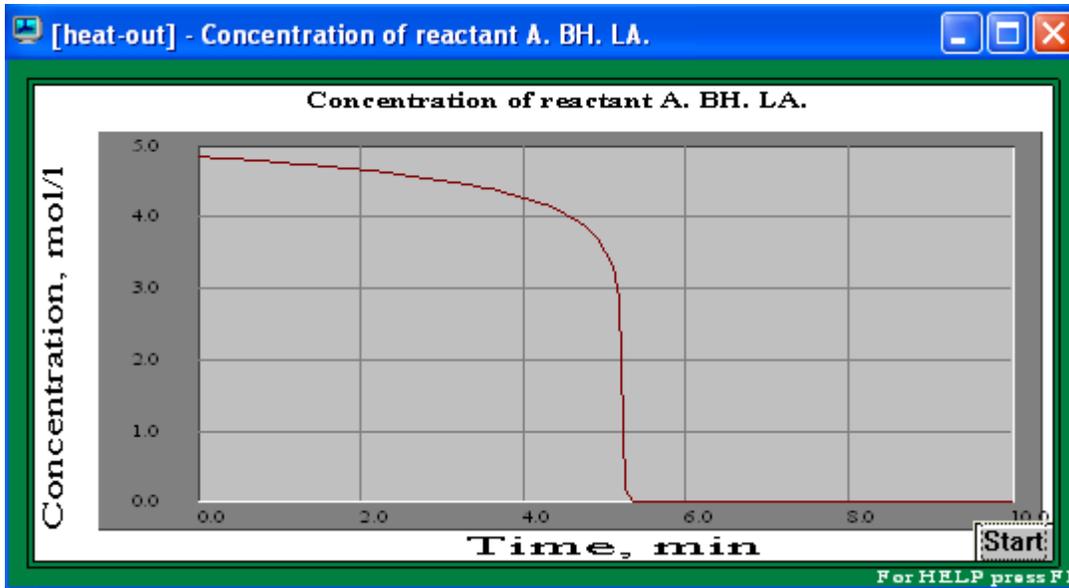
Figure 29. Concentration of reactant A. BH. LA. The heating stage is 5 min.

These results show that this scenario, ensuring greater process safety, is at the same time capable of completing the reaction. The duration of the cooling stage is now about 5 minutes, and the total reaction time is about 10 minutes.

Conclusion:

You have thus confirmed the suitability of your equipment to your exothermal process, and found an optimal process regime. It really means that VisiMix® software provided improvement of the Inherently Safer Design (***ISD***) of your reactor.