VISIMIX TURBULENT. COOLING OF A REACTOR WITH HALF-PIPE COIL FOR PRODUCTION OF PROPYLENE GLYCOL. RELEASE OF REPORT.

This example demonstrates VisiMix capabilities in simulating industrial processes controlled by exothermal reaction. An example of such a process is borrowed from the book of H. Scott Fogler, *Elements of Chemical Reaction Engineering*, 2nd ed. (Prentice-Hall, Inc. 1992), pp. 400 - 405, *Examples 8-4 and 8-5*.

Problem description:

Propylene glycol (**PG**) is produced by the hydrolysis of propylene oxide (**PO**). The reaction takes place at room temperature when catalyzed by sulfuric acid.

$$PO + H_2O \longrightarrow PG$$

In accordance with the technological requirements, 2500 lb/h (43.03 lb-mole/h) of **PO** is fed to the reactor. The feedstream consists of

(1) a mixture of equal volumes of **PO** (46.62 ft³/h) and **methanol** (46.62 ft³/h), and (2) **water** containing 0.1 mass percent of H_2SO_4 . The volumetric flow rate of **water** is 233.1 ft³/h, which is 2.5 times **methanol** - **PO** flow rate. The corresponding molar feed rates of **methanol** and **water** are 71.87 and 802.8 lb-mole/h, respectively. The inlet temperature of all feedstreams is 75°F. The reaction under consideration is first-order in **PO** concentration, and apparent zero-order in excess of water with the specific reaction rate

$$k = A e^{-E/RT} = 16.96 * 10^{12} (e^{-32400/RT}) h^{-1}$$
 (1)

In this equation, E is measured in Btu/lb-mole.

The process has an important operating constraint. The temperature of the mixture must not exceed 130°F because of the low boiling point of **PO**.

The task is to determine whether this process can be carried out in a glass-lined continuos-stirred 300-gal reactor.

You must design an appropriate jacketed tank corresponding to this capacity and to the temperature limit above, perform simulation and determine the **PO-PG** conversion.

Preliminary considerations

In order to enter the required initial data, you must perform the following calculations:

Volume of media is $300 \text{ gal} = 40.1 \text{ ft}^3$.

All flow rate values are presented below in Table 1.

Material	Volumetric Flow Rate, ft ³ /h	Mole Flow Rate, Ib-mole/h
PO	46.62	43.03
Methanol	46.62	71.87
Water	233.1	802.8

Table 1. Flow rates.

Total volumetric flow rate: 46.62 + 46.62 + 233.1 = 326.34 ft³/h;

VisiMix considers exothermal second order reactions only. It means that the *A* factor, equal to $16.96 * 10^{12}$ (see Eq. 1 for specific reaction rate *k*) and corresponding to the case when the reaction is first-order with regard to the **PO** concentration, and apparent zero-order with regard to water excess, must be transformed into A_{new} .

Initial concentration of reactant **A** (**PO**): 43.03 lb-mole/h / 326.34 ft³/h = 0.1319 lb-mole/ft³ (2.1128 mole/liter);

Initial concentration of reactant **B** (water): 802.8 lb-mole/h / 326.34 $ft^3/h = 2.46$ lb-mole/ft³ (39.404 mole/liter);

 $A_{new} = A / 2.46 = 16.96 * 10^{12} / 2.46 = 6.894 * 10^{12}$ ft³/ lb-mole/h (1.1964*10⁸ liter/mole/sec).

Heat effect of reaction: 36540 Btu/lb-mole (85000 J/mole).

The process is simulated as a steady state of the transient occurring in the following conditions. The reactor is filled with water which is then expelled by two components: reactant **A** (**PO** with flow rate equal 46.62 ft³/h) and reactant **B**, which is actually a mixture of **methanol** (46.62 ft³/h) and **water** containing 0.1 mass percent of **H**₂**SO**₄ (233.1 ft³/h). The properties of reactant **B** are close to those of ordinary water, and therefore you should enter water properties in the input tables.

The Solution:

The general sequence of operations is as follows: you must start a new project file for your case, select your equipment from the graphical menus, enter the initial data requested by the program, and then select the parameter/s for calculation from the **Calculate** menu. The program will then request additional data required for the modeling, and when all this data has been entered, you will obtain the result, presented as a table or a graph. In your case of a continuous flow reactor, you must select **Heat transfer. Continuous Flow (CF)** option in the **Calculate** menu, and calculate the following parameters: **Media temperature**, to ensure that the temperature of the mixture does not exceed 130°F, and **Concentration of reactant A (PO)** required to calculate the conversion value.

After installing **VisiMix**, the main menu shown in Figure 7-1 appears. Select **Project-New**.



Figure 7-1. VisiMix main menu.

A dialogue shown in Figure 7-2 will appear. Enter a name for your project, for example **PG-Production**, and save it in any convenient directory, for example, **tutorial**.

🛃 Enter a pro	oject name		×
Save in: 📜	Tutorial		* == •
Name 🔺		•	Date modified
🛛 👢 Jan14_20	14		1/14/2014 6:1
dissolution	.VSM		1/23/2014 6:5
heat-in.VS	м		1/23/2014 9:4
heat-out1	.VSM		1/25/2014 12:
heat-out2	.VSM		1/25/2014 12:
hydrod.V5	SM		1/16/2014 9:3
•			▶
File name:	PG-Production1.VSM		Save
Save as type:	VisiMix Project Files (*.vsm)	•	Cancel

Figure 7-2. 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 with elliptical bottom and half-pipe coil jacket, and it will appear in the **Current choice** window on the right (Figure 7-3).



Figure 7-3. VisiMix graphic tanks selection.

Click **OK** to confirm your choice, and TANK WITH ELLIPTICAL BOTTOM input table with the selected tank diagram appears. Enter the **Inside diameter**, **Total tank height**, and **Volume of media** for your available 300-gal reactor. The **Total volume** and **Level of media** will be calculated by the program and entered automatically (Figure 7-4). Click **OK** to confirm your input.

C:\VisiMix\Tutorial\PG-Produ	uction1.VSM	X
TANK WITH ELL	IPTICAL BOTTOM	
Inside diameter	1200 mm 💌	
Total tank height	1300 mm 💌	
Total volume	1357 I 💌	1300
Level of media	1104 mm 💌	
Volume of media	300 gal 💌	< 1200 >
OK Cancel	Choose new tank Print	Help

Figure 7- 4. Entering tank data.

After you click **OK**, the **Baffle types** menu with different baffles (without baffles, two types of flat baffles and two types of tubular ones) appears. To choose the required baffle type, click on the appropriate baffle diagram. Let us select a flat baffle attached to the wall (Flat baffle 1), and it will appear in the **Current choice** window on the right (Figure 7-5). Click **OK** to confirm your choice



Figure 7-5. VisiMix graphic baffle selection.

Now you have to enter all your baffle data in FLAT BAFFLE-1 input table that appears (Figure 7-6).

C:\VisiMix\Tutorial\PG-Produ	ction1.VSM			×
FLAT	BAFFLE-1			
Number	4]		
Width	100	mm		8
Length	1000	mm		13
Dist. from bottom	300	mm	Ø 1200	I
Angle to radius (fi)	0	deg 💌	x fi	
OK Cancel	Choose new baffle	Print		Help

Figure 7-6. Entering baffle data.

Click **OK** to confirm your input, and **Impeller types** menu appears. Choose your singlestage pitched paddle impeller by clicking on the appropriate diagram, and on the **single** option in the **Current choice** window on the right (Figure 7-7). Click **OK** to confirm your choice.



You will now be asked to complete PITCHED PADDLE input table (Figure 7-8).

Figure 7-7. VisiMix graphic impeller selection.

C:\VisiMix\Tutorial\PG-Produ	ction1.VSM	X
PITCHED	PADDLE	
Tip diameter	600 mm 💌	
Number of blades	4	
Pitch angle	45 deg 💌	
Width of blade	120 mm 💌	
Dist. from bottom	300 mm 💌	
Rotational speed	180 Rpm 💌	
Motor power	6 KW 💌	< ^{Ø 1200} >
Pumping direction	down 💌	
OK Cancel Ch	oose new impeller Print	Help

Figure 7-8. Entering impeller data.

Click **OK** to confirm your input, and TANK HEAT TRANSFER GENERAL DATA input table appears (Figure 7-9). Note that for your single-sectioned jacket, only those parameters that refer to the lower jacket section will be active.

The completed table will include the following data regarding the jacketed tank design:

Tank head type	Elliptical
Jacket covers bottom:	Yes
Number of jacket sections:	1
Height, H _{low} (mm):	1000

VisiMix\Tutorial\PG-I	Production1.	VSM				
TANK HEAT TRA	ANSFER GENE	ERAL DATA				Help
Tank head type Jacket covers bottom Number of jacket sections Lower section Distance from bottom Height Hlow Heat transfer area for lower section according If unknown, enter 0*	Elliptical YES 1 1000 0	▼ ▼ ▼ mm mm sq.m	V	HIOW		300
Upper section Distance between two sections Height Hup Heat transfer area for upper section according If unknown, enter 0 * Connection of jackets		mm mm sq.m			Ø 1200	
* In this case heat tran	isfer area will b VisiMix	e e∨aluated	by	ОК	Cancel	Print

Figure 7-9. Entering general jacket characteristics.

You will then be asked to enter average properties of media including DENSITY AND TYPE OF MEDIA input table (Figure 7-10a) and AVERAGE VISCOSITY OF MEDIA input table (Figure 7-10b).

C:\VisiMix\Tutorial	PG-Production1.VSM	x
	DENSITY AND TY	PE OF MEDIA
, Average density	1000 kg/cub.m	I
	TYPE OF M	EDIA
 Newtonian 	Power-law non-Newtonian	Carreau non-Newtonian
τ=μ * γ	$\tau = \tau_{\circ} + K * \gamma^{n}$ $\mu = \tau_{\circ} * \gamma^{-1} + K * \gamma^{n-1}$	$\frac{\mu^{-\mu_{\min}}}{\mu_{\max}-\mu_{\min}} = \left[1 + (\lambda * \gamma)^2\right]^{\frac{n+1}{2}}$
OK	Cancel Print	Help

Figure 7-10a. Density and type of media.

C	\VisiMix\Tutorial\PG-Production1.VSM
	AVERAGE VISCOSITY OF MEDIA
	Dynamic viscosity 0.001 Pa*s \checkmark Kinematic viscosity 1e-06 sq.m/s \checkmark where τ -shear stress, Pa; μ -dynamic viscosity, Pa*sec; γ -shear rate, 1/sec;
	OK Cancel Print Help

Figure 7-10b. Average viscosity of media.

After this table has been completed, the diagram of your mixing system corresponding to the data you have entered appears (Figure 7-11). We recommend closing this window before proceeding to calculations. If at any stage of your working on a project you will need the diagram of your apparatus, click on the quick access button in the upper screen bar.



Figure 7-11. Drawing of apparatus.

Now when all basic initial data has been entered, you can start the calculations. For your reactor, you must select **Heat Transfer. Continuous Flow (CF) - Liquid agent (LA)** option in the **Calculate** menu. As mentioned before, you need to calculate **Media temperature** and **Concentration of reactant A**. Click on **Media temperature**. For calculating this parameter, additional data is needed, and the program will request it by invoking the appropriate input tables. First you will be asked to complete HEAT TRANSFER. CHEMICAL REACTION DATA AND TEMPERATURE LIMITS (Figure 7-12). Upper temperature limit is 130° F as mentioned above.

C:\VisiMix\Tutorial\PG-Pro	oduction1.VSM			×
HEAT TRAN	NSFER. CHEMIC	AL REACTION DA	ATA AND	TEMPERATURE LIMITS
Will you enter reaction kinetics? Arrhenius constant Energy of activation Lower limit of temperature Upper limit of temperature Heat effect of reaction	YES 1.196e+08 7.538e+04 15 130 8.501e+04	V(mol*sec) J/mol C 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 /(b*mol)/*F is universal gas constant, T is absolute temperature.
ОК	Cancel	Print		Help

Figure 7-12. Heat transfer. Process temperature limits

Then TANK SHELL CHARACTERISTICS input table appears (Figure 7-13). Select your tank shell material, wall thickness, and thermal resistance of fouling. The latter can be found in the table **Thermal resistance of fouling** in the **APPENDIX** of the **Help** section. For water, which is an in-jacket thermal agent in your example, the recommended value is $0.00023 \text{ (m}^2 \cdot \text{K})/\text{W}$.

The next table you will be asked to complete is HALF - PIPE COIL JACKET. SPECIFIC CHARACTERISTICS (Figure 7-14)

C:\VisiMix\Tutorial\PG-Proc	luction1.VSM X
TANKS	SHELL CHARACTERISTICS
Material	Steel glass lined
Wall thickness	8 mm 💌
Thermal resistance of fouling	0.00023 (m ^{2*} K)/W
Tank mass (without drive) If unknown, enter 0 *	0 kg 💌
ок с	ancel Print Help
* In this case tank mass will be	e evaluated by VisiMix

Figure 7-13. Tank shell characteristics.

HALF-F	PIPE COIL JA	ACKET. SPECIFIC CHAP	ACTERISTICS.
Lower section			
Pipe diameter, lower section, d	80	mm 💌	
Distance between coils, l	200	mm 💌	
Number of starts	2		
Upper section			_ ↓ ♪
Pipe diameter, upper section, d		mm 🔽	
Distance between coils, l			
Number of starts			

Figure 7-14. Half-pipe coil jacket. Specific characteristics.

After this table has been completed, HEATING / COOLING LIQUID AGENT IN JACKET input table appears (Figure 7-15), and then HEAT TRANSFER PROPERTIES OF THE MEDIA input table (Figure 7-16)..

C:\VisiMix\Tutorial\PG-Produ	C:\VisiMix\Tutorial\PG-Production1.VSM						
HEATING / COOLING LIQUID AGENT IN JACKET.							
Heating/cooling agent	Water						
Inlet temperature	30 °C 🔽						
Flow rate of heat transfer agent	8 cub.m/h 🔽						
in lower jacket	· · _						
Flow rate of heat transfer agent in upper jacket	cub.m/s						
OK Cancel	Print Help						
Operating temperature range: 5 - 204°C [41 - 400°F]							
Properties of the agent density1000 kg/m ^o [62.4 lbm/tt ^o] enset finance 4 lbm/tt ^o]							
thermal conductivity0.603 W/m*K [0.348 (Btu*ft)/(h*ft**F)] dynamic viscosity at 100°C/212°E) 0.000284 Pa*sec [0.284 cP]							
aynanne viscosity at 100 c(c12 1)0.000204 Pa sec [0.204 CF]							

Figure 7-15. Heating/cooling liquid agent in jacket.

C:\VisiMix\Tutorial\PG	-Production1.VSM				×
	HEAT TRANSFER F	PROPERTIES OF THE	MEDIA		
Media	Water solution	V			
	PARAMETER		TE	MPERATURE	
Average density	1000 kg/c	ub.m	- 20	0°	•
Dynamic viscosity	0.001	3	▼ 20	0°	⊡
Specific heat	4182 J/(k	g*K) ·	▼ 20	°C	
Heat conductivity	0.6 W/(r	n*K)	✓20).	
ОК	Cancel	Print		Help	

Figure 7-16. Heat transfer properties of the media.

The last table you will be asked to complete is CONTINUOUS FLOW PROCESS. HEAT TRANSFER SPECIFIC DATA. The completed table is shown in Figure 7-17.

C:\VisiMix\Tutorial\F	PG-Production	1.VSM				×
	CONTINUOUS	FLOW PROCESS. HE	AT TRANSFER SP	PECIFIC DATA.		
Initial temperature in	40					
the tank	40					
Temperature of inlet flow	30	°C 💌	Inlet flow rate	0.00257	cub.m/s	•
Initial concentration of reactant A in the tank	0	Ib.mol/cub.ft 🔻	Density of inlet	1000	kg/cub.m	-
Initial concentration of	,		110W			_
reactant B in the tank	39.4	mol/liter	inlet flow	4182	J/(kg*K)	•
Concentration of reactant A in the inlet flow	2.113	mol/liter 💌	Average rate of heat release (consumption)		W	V
Concentration of reactant B in the inlet flow	39.4	mol/liter 💌	Simulation time	60	min	•
ОК	Cancel	Print			Help	

Figure 7-17. Continuous flow process. Heat transfer specific data.

Now, when you have entered all the required parameters of your equipment and process, VisiMix will start calculations. In a very short time, a graph of **Media temperature. CF. LA.** appears (Figure 7-18). Click on **Start** to start the simulation.

🖳 [PG-Prod	luction1] - Med	lia temperature. C	F. LA.					
			\mathbf{Me}	dia temper	ature. CF. I	A .		
U	52.0							
0	50.0							
່ຍົ	48.0							
E E	46.0							
뮾	44.0							
Ľ,	42.0							
b	40.0							
Ē	40.0							
ē	38.0							
H	36.0	0.0	10.0	20.0	30.0	40.0	50.0	
				Tim	ıe, m	lin		Start
							For HELF	press F1

Figure 7-18. Media temperature. CF. LA.

From this graph, you can see that your process requirement is met: the temperature does not reach 130° F (54.55 °C).

You must now check the conversion factor. The conversion is estimated as concentration of **PG** divided by concentration of **PO**, that is the difference between the initial concentration of reactant A in the inlet flow and the final concentration of reactant A as calculated by VisiMix, divided by the initial concentration of reactant A in the inlet flow.

To obtain final concentration of reactant A, click on **Last menu** in the main menu and select **Concentration of reactant A. CF. LA.** You will obtain a graph shown in Figure 7-19. Click on **Start** to start the simulation, and from the curve that appears take the concentration value (0.85 in your case). Therefore, the conversion factor can be calculated as follows:

$$\frac{C_{POin} - C_{PO}}{C_{POin}} = \frac{2.113 - 0.85}{2.113} = 0.6$$

where C_{POin} is concentration of **PO** (reactant A) in the inlet flow, and C_{PO} is final concentration of **PO** (reactant A) in the reactor.



Figure 7-19. Concentration of reactant A. CF. LA.

If you want to check the effect of other process parameters, click on **Last menu**, and select the required parameters. Some of the calculated results are shown below in Figs 7-20—7-22.



Figure 7-20. Concentration of reactant B. CF. LA.



Figure 7-21. Outlet temperature of LA in lower jacket. CF.

G-Production1] - Pressure head on the jacket, max		
PRESSURE HEAD C	ON THE JACKET, MAX	
Parameter name	Units	Value
Pressure head on lower jacket	N/sq.m	14000
Pressure head on upper jacket	N/sq.m	0

Figure 7-22. Pressure head on the jacket, maximum value.

You have thus designed a glass-lined continuos-stirred 300-gal reactor, checked its suitability to your process, simulated your process in this reactor and determined the **PO-PG** conversion.

Now let us see how to prepare a VisiMix **Report** for your project, which accumulates the initial data and calculated results in a file of a standard HTML format. All graphs, in addition to a graph form, are presented in a standard tabular format. This enables you to plot and process your data in any way you wish using, for example, EXCEL, or QUATTRO PRO.

Selecting **Report** at any stage of working on a current project invokes a submenu, which is identical to the **Calculate** submenu (Figure 7-23).

🛃 VisiMix Turbulent (release 11a)	
Project Edit input Calculate Suppleme	nts Last menu Last input table Window View Help
New Open	
Clone	
Project comments	
Save	
Save As	
Report Print	Hydrodynamics Turbulence
1 C:\VisiMix\Tutorial\PG-Production1.VSM 2 C:\VisiMix\Tutorial\PG-Production.VSM 3 C:\VisiMix\Tutorial\heat-out2.VSM 4 C:\VisiMix\Tutorial\heat-out1.VSM	Single-phase liquid mixing Continuous flow dynamics Batch reaction/blending Semibatch reaction Continuous flow reaction
Exit A	Liquid-solid mixing Liquid-liquid mixing Gas dispersion and mass transfer Liquid-solid mass transfer
	Heat Transfer - Continuous flow
	Heat Transfer - Batch process Vapor agent Heat Transfer - Semibatch process Heat Transfer. Fixed temperature regime
	Mechanical calculations of shafts
	Supplements

Figure 7-23. The Report menu.

Choose your calculation option, i.e. **Heat transfer. Continuous flow, Liquid agent**, and enter the report name in the **Save as** dialogue that appears (Figure 7-24). VisiMix will create a report including relevant initial data and the results of the calculations.

🛃 Save As			×
Save in: 📜	Tutorial	▼ ← € (* ⊞▼
Name 🔺		•	 Date modified
🛛 👢 Jan14_20	14		1/14/2014 6:11 Pl
•			Þ
File name:	Report_PG-Production1.VSM		Save
Save as type:	VisiMix Report Files (*.HTM)	•	Cancel

Figure 7-24. Entering a name for the Report.

On completing the report, VisiMix issues a message (Figure 7-25).

Information	×
REPORT COMPLETED !	

Figure 7-25. Message on the completion of the Report.

Click **OK**. Your report is formed as a file with a **.htm** extension, and you may open, edit and print this file from Microsoft Internet Explorer.

Some of the results for this example as they appear in the Report are shown below.

THE RESULTS

TABLE OF RESULTS

Parameter name	Units	Value
Heat transfer area. Lower section	sq.m	5.02
Active heat transfer area. Lower section	sq.m	4.37
Pressure head on lower jacket	N/sq.m	14000
Liquid velocity, lower jacket	m/s	0.442

Media temperature. CF. LA.

Argument	Function	Argument	Function	Argument	Function
0	40	2.5	37.6644	5	36.9941
7.5	37.1106	10	37.6492	12.5	38.4272
15	39.3414	17.5	40.3296	20	41.3523
22.5	42.3823	25	43.399	27.5	44.3864
30	45.3304	32.5	46.2196	35	47.0428
37.5	47.7915	40	48.4604	42.5	49.0462
45	49.5487	47.5	49.9715	50	50.3201
52.5	50.6023	55	50.8262	57.5	51.0015