Solution of a System of ODEs with POLYMATH and Excel, Parametric Studies with Excel

The canonical form of a system of *n* simultaneous first-order ordinary differential equations ODE with specified initial values (initial value problem) is:

$$\frac{dy_1}{dx} = f_1(y_1, y_2, \ldots y_n, x) \qquad y_1(x_0) = y_{1,0}$$

$$\frac{dy_2}{dx} = f_2(y_1, y_2, \ldots y_n, x) \qquad y_2(x_0) = y_{2,0}$$

$$\vdots \qquad\qquad\qquad\qquad \vdots$$

$$\frac{dy_n}{dx} = f_n(y_1, y_2, \ldots y_n, x) \qquad y_n(x_0) = y_{n,0}$$

where x is the independent variable and $y_1, y_2, \ldots y_n$ are dependent variables

Adiabatic Operation of a Tubular Reactor for Cracking of Acetone

The irreversible, vapor-phase cracking of acetone (A) to ketene (B) and methane (C) that is given by the reaction:

$$CH_3COCH_3 \rightarrow CH_2CO + CH_4$$

is carried out adiabatically in a tubular reactor. The reaction is first order with respect to acetone and the specific reaction rate can be expressed by

$$\ln k = 34.34 - \frac{34222}{T}$$

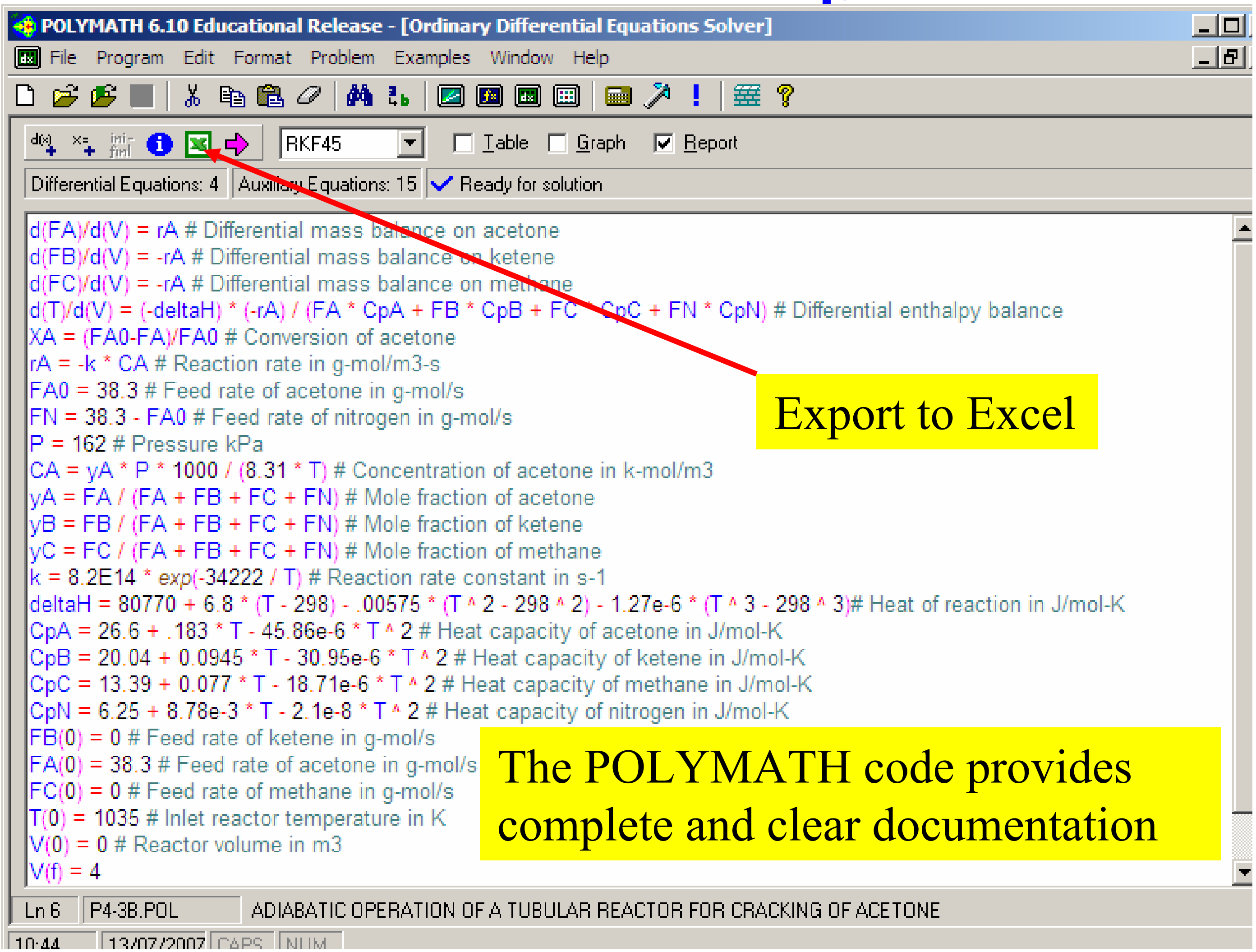
The acetone feed flow rate to the reactor is F_A mol/s, the inlet temperature is $T = 1150$ K and the reactor operates at the constant pressure of $P = 162$ kPa (1.6 atm). The volume of the reactor is $V = 4$ m^3. Inert gas (nitrogen) is fed at the rate of F_N mol/s.

Adiabatic Operation of a Tubular Reactor for Cracking of Acetone - Assignments

(a) Calculate the flow-rates (in mol/s) and the mole fractions of acetone, ketene and methane along the reactor for the case where pure toluene is being fed at the rate of F_A = 38.3 g-mol/s. Use Polymath to calculate and plot the conversion and reactor temperature (in K) versus volume.

(b) The conversion in the reactor in part (a) is very low in adiabatic operation because the reactor content cools down very quickly. It is suggested that feeding nitrogen along with the acetone might be beneficial in maintaining a higher temperature. Compare the final conversions and temperatures for the cases where 28.3, 18.3, 8.3, 3.3 and 0.0 mol/s nitrogen is fed into the reactor (the total molar feed rate is 38.3 mol/s in all the cases).

Adiabatic Operation of a Tubular Reactor for Cracking of Acetone – Model Equations



Adiabatic Operation of a Tubular Reactor for Cracking of Acetone – Solution for F_A = 38.3 mol/s

POLYMATH 6.10 Educational Release - [Differential Equations Solution #1]

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POLYMATH Report
Ordinary Differential Equations

ADIABATIC OPERATION OF A TUBULAR REACTOR F

Calculated values of DEQ variables

	Variable	Initial value	Minimal value	Maximal value	Final value
1	CA	18.83535	12.68959	18.83535	12.68959
2	CpA	166.8786	154.9084	166.8786	154.9084
3	CpB	84.69309	80.3113	84.69309	80.3113
4	CpC	73.04238	67.86058	73.04238	67.86058
5	CpN	15.3148	14.20092	15.3148	14.20092
6	deltaH	7.876E+04	7.876E+04	7.977E+04	7.977E+04
7	FA	38.3	28.44647	38.3	28.44647
8	FA0	38.3	38.3	38.3	38.3
9	FB	0	0	9.853527	9.853527
10	FC	0	0	9.853527	9.853527
11	FN	0	0	0	0
12	k	3.580818	0.0344545	3.580818	0.0344545
13	P	162.	162.	162.	162.
14	rA	-67.44594	-67.44594	-0.4372133	-0.4372133
15	T	1035.	907.5422	1035.	907.5422
16	V	0	0	4.	4.
17	XA	0	0	0.2572723	0.2572723
18	yA	1.	0.5907454	1.	0.5907454
19	yB	0	0	0.2046273	0.2046273
20	yC	0	0	0.2046273	0.2046273

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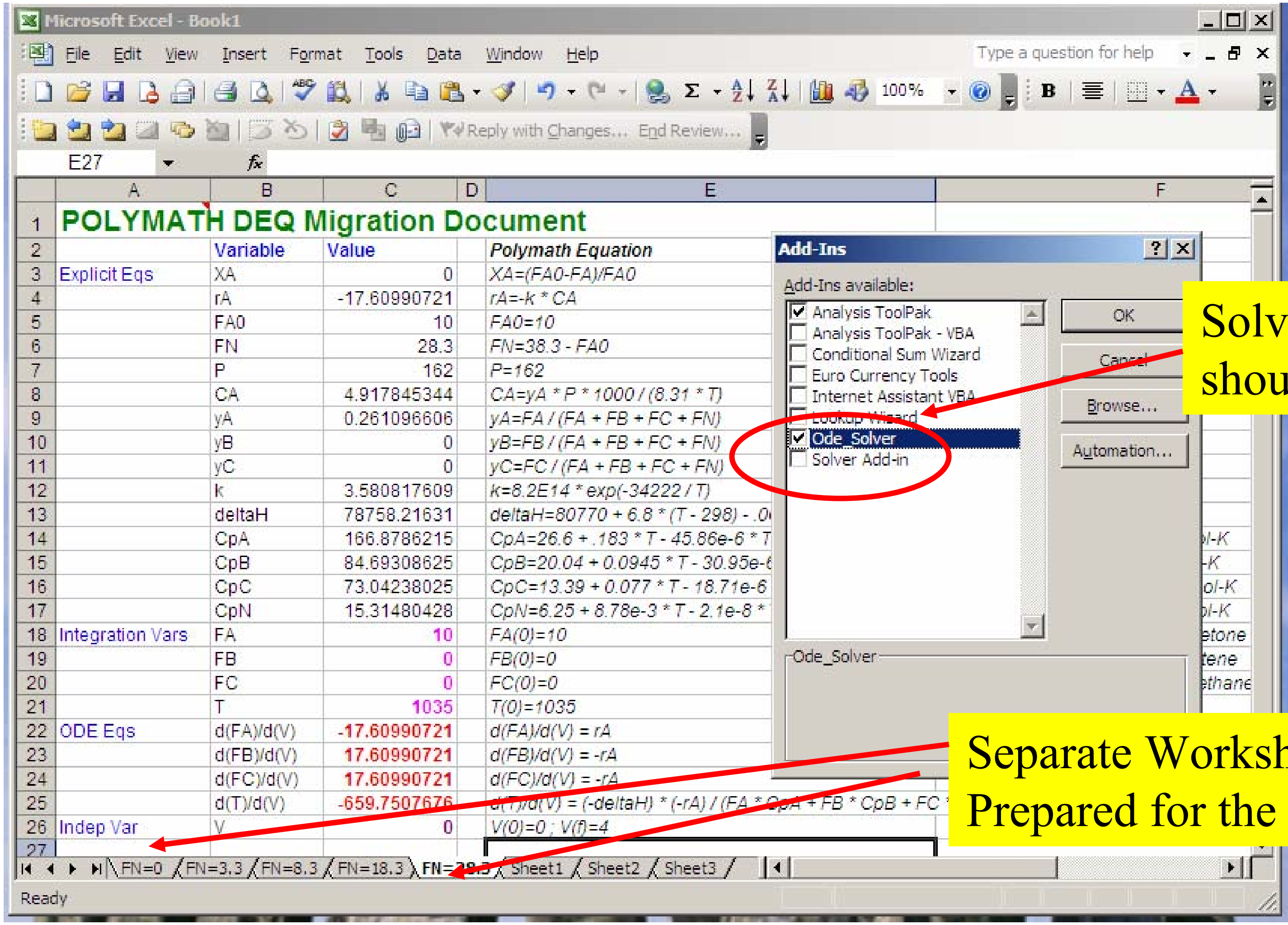
Drop of ~120 K in the temperature reduces the reaction rate by two orders of magnitude

Low conversion of the reactant

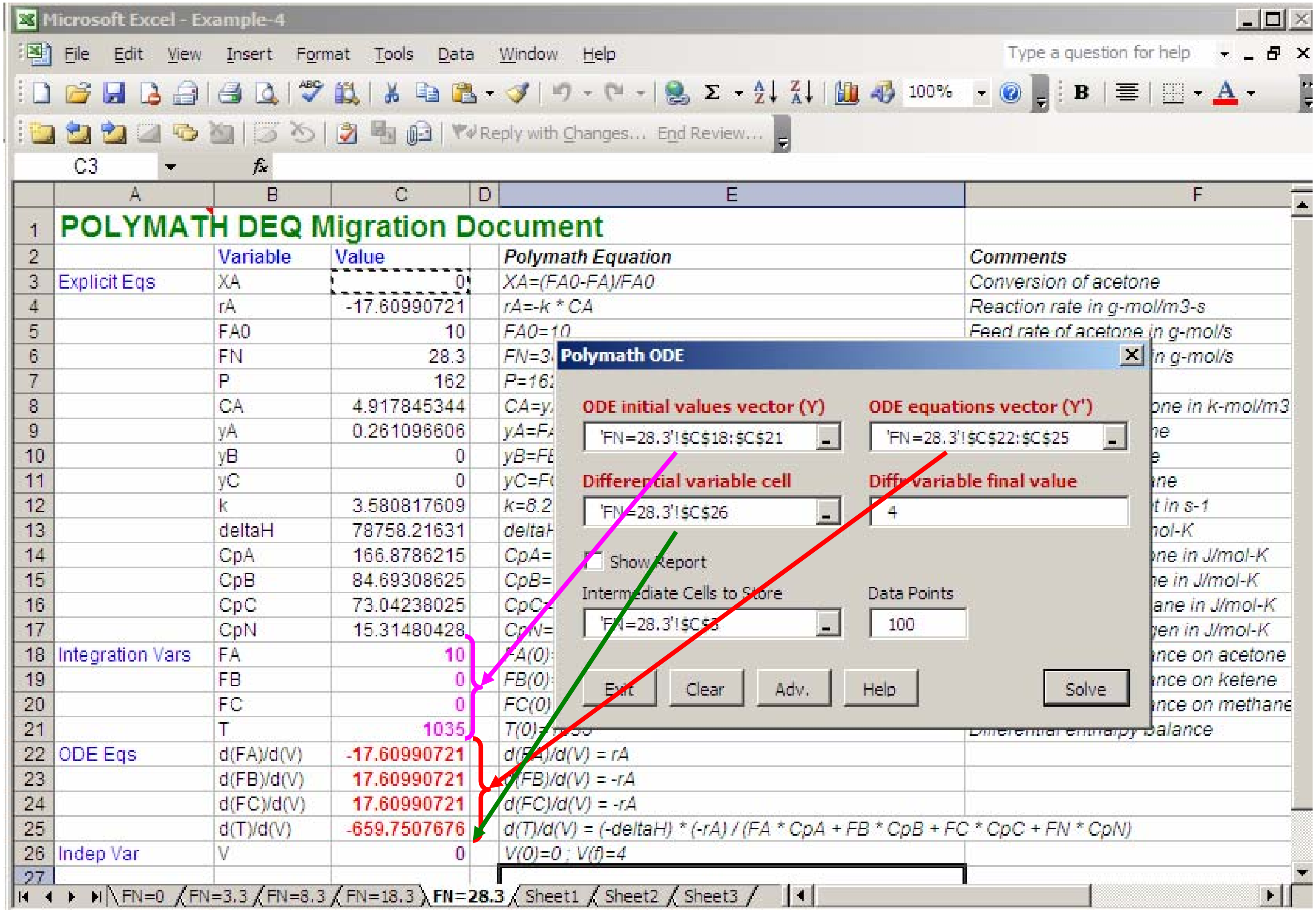
Adiabatic Operation of a Tubular Reactor – Exporting to Excel and Adding the ODE Solver



Solver Add-In should be removed

Separate Worksheets are Prepared for the Various Cases

Adiabatic Operation of a Tubular Reactor – ODE Solver Add In Communication Box



Adiabatic Operation of a Tubular Reactor – Comparison of results for F_N = 0 and F_N = 28.3

Microsoft Excel - Example-4

POLYMATH DEQ Migration Document

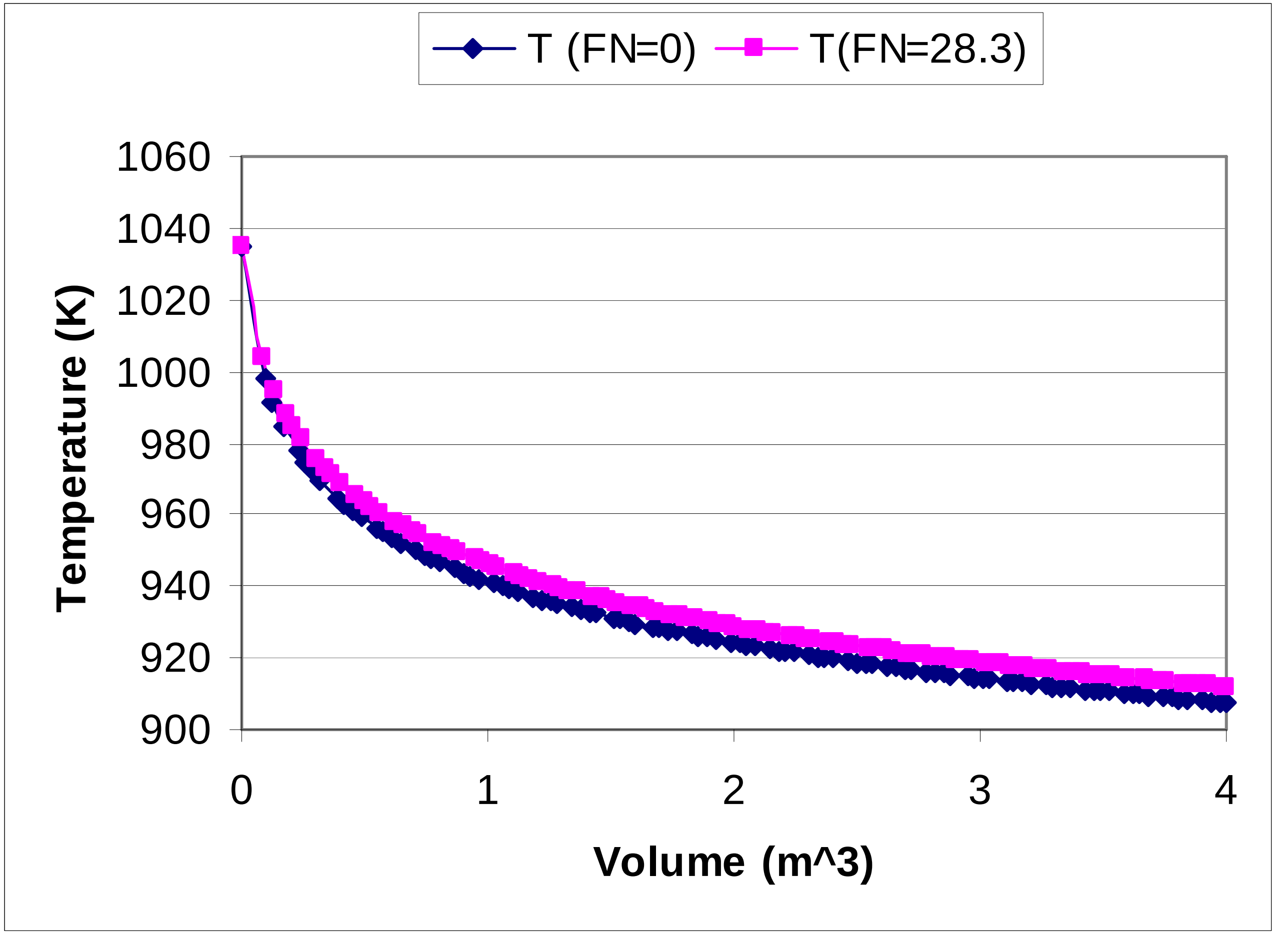
	A	B	C	D	E	F
2		Variable	Value	Value	uation	Comments
3	Explicit Eqs	XA	0.313552401	0.257272258	/FA0	Conversion of acetone
4		rA	-0.145866418	-0.437213285		Reaction rate in g-mol/m3-s
5		FA0	10	38.3		Feed rate of acetone in g-mol/s
6		FN	28.3	0	0	
7		P	162	162		
8		CA	3.541783023	12.68958732	000 / (8.3	
9		yA	0.165666446	0.590745352	FB + FC + F	
10		yB	0.075672363	0.204627324	FB + FC + F	
11		yC	0.075672363	0.204627324	FB + FC + F	
12		k	0.041184459	0.034454492	xp(-34222	
13		deltaH	79744.527	79773.92861	0 + 6.8 * (T -	
14		CpA	155.3379823	154.9084155	183 * T - 45.	
15		CpB	80.47607044	80.3112995	0.0945 * T -	
16		CpC	68.04592572	67.86057679	0.07 * T -	
17		CpN	14.2386407	14.2009238	3.78e-3 * T -	
18	Integration Vars	FA	6.864475993	28.44647253		Differential mass balance on acetone
19		FB	3.135524007	9.853527468		Differential mass balance on ketene
20		FC	3.135524007	9.853527468		Differential mass balance on methane
21		T	911.8567009	907.5421516		Differential enthalpy balance
22	ODE Eqs	d(FA)/d(V)	-0.145866418	-0.437213285	A	
23		d(FB)/d(V)	0.145866418	0.437213285	rA	
24		d(FC)/d(V)	0.145866418	0.437213285	rA	
25		d(T)/d(V)	-6.011513678	-5.945205114	eltaH) * (-rA) / (FA * CpA + FB * CpB + FC * CpC + FN * CpN)	
26	Indep Var	V	4	4	4	

FN=0 | FN=3.3 | FN=8.3 | FN=18.3 | FN=28.3 | DEQ Solution (1) | Sheet1 | Sh

Ready

No significant change in the temperature profile and the conversion occurs because of the addition of the inert gas.

Adiabatic Operation of a Tubular Reactor – Comparison of results for $F_N = 0$ and $F_N = 28.3$



Adiabatic Operation of a Tubular Reactor – Comparison of results for $F_N = 0$ and $F_N = 28.3$