A Case Study on Synthesis of Ammonia in Cryogenic Process

Problem Statement

Ammonia has to be synthesized from a mixture of N_2 (24%), H_2 (74%), CH_4 (1%), and Ar (1%). The mixture is flowing at 5000 kmol/hr, 50 °C, and 90 bar. The equilibrium reactor at 50 °C and zero pressure drop will be modelled using the concept of Gibbs Free Energy Minimization. The outlet of the reactor will be depressurized at 15 bar using a valve and the flashed at -35 °C (with zero pressure drop). Liquid outlet of the flash is the main product line which contains Ammonia. The vapour outlet of the flash tank is passed through a membrane separator to separate 90% of mixture of H_2 and N_2 for recycling back to the feed line after appropriate pressure (isentropic compressor with 90% isentropic and 80% mechanical efficiency) and temperature correction. Remaining 10% is purged.

1. Employ Idean, NRTL, and Peng Robinson property methods and compare their performance in predicting ammonia production.
2. The plant is optimized for ammonia production with its quality constraint of 99.8% purity. The operating temperature of flash tank and reactor will be used for that purpose.

Major steps and results of Aspen Plus Simulation are given below,

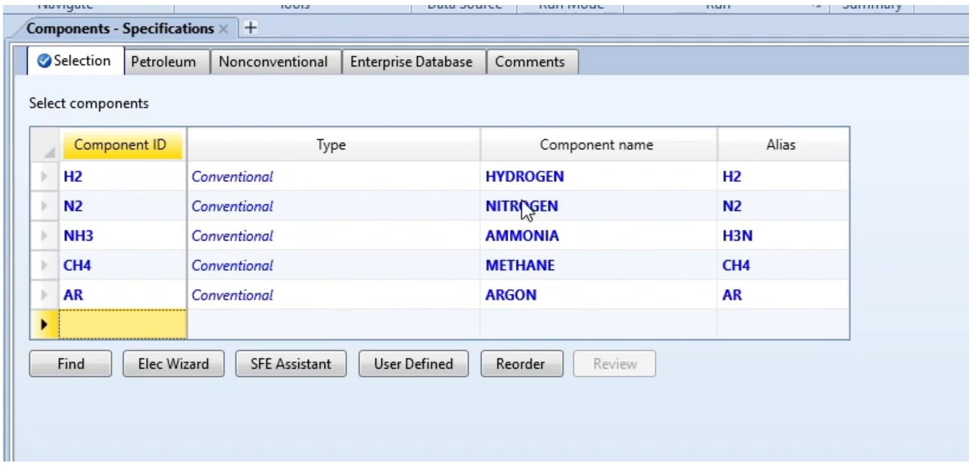

Fig: Component Selection

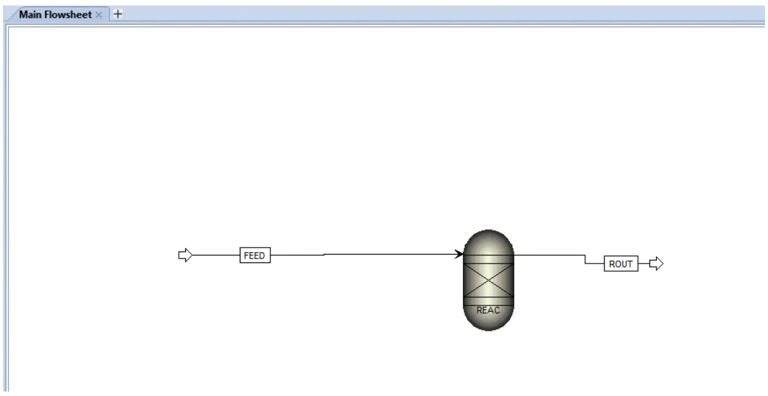

Fig: Basic Flowsheet for Equilibrium Reactor

	Units	FEED	ROUT	ROUT	ROUT
− Mole Flows	**kmol/hr**	**5000**	**2600.31**	**2600.31**	**2600**
H2	kmol/hr	3700	100.467	100.467	100.004
N2	kmol/hr	1200	0.155693	0.155693	0.00124707
NH3	kmol/hr	0	2399.69	2399.69	2400
CH4	kmol/hr	50	50	50	50
AR	kmol/hr	50	50	50	50
− Mole Fractions					
H2		0.74	0.0386366	0.0386366	0.0384629
N2		0.24	5.98748e-05	5.98748e-05	4.79643e-07
NH3		0	0.922847	0.922847	0.923075
CH4		0.01	0.0192285	0.0192285	0.0192308
AR		0.01	0.0192285	0.0192285	0.0192308
− Mass Flows	**kg/hr**	**43874.5**	**43874.5**	**43874.5**	**43874.5**
H2	kg/hr	7458.76	202.53	202.53	201.596
N2	kg/hr	33616.2	4.3615	4.3615	0.0349349
NH3	kg/hr	0	40868	40868	40873.3
CH4	kg/hr	802.138	802.138	802.138	802.138
AR	kg/hr	1997.4	1997.4	1997.4	1997.4
− Mass Fractions					
H2		0.170002	0.00461611	0.00461611	0.00459483
N2		0.76619	9.94087e-05	9.94087e-05	7.96246e-07
NH3		0	0.931477	0.931477	0.931596
CH4		0.0182826	0.0182826	0.0182826	0.0182826
AR		0.0455253	0.0455253	0.0455253	0.0455253

Fig: Stream Results for Different Property Methods, the 1st column is for Ideal, 2nd for NRTL and 3rd for Peng Robinson

For these results we can say that Peng Robinson is the best property method for our case study because it gives most appropriate results compared to Ideal and NRTL.

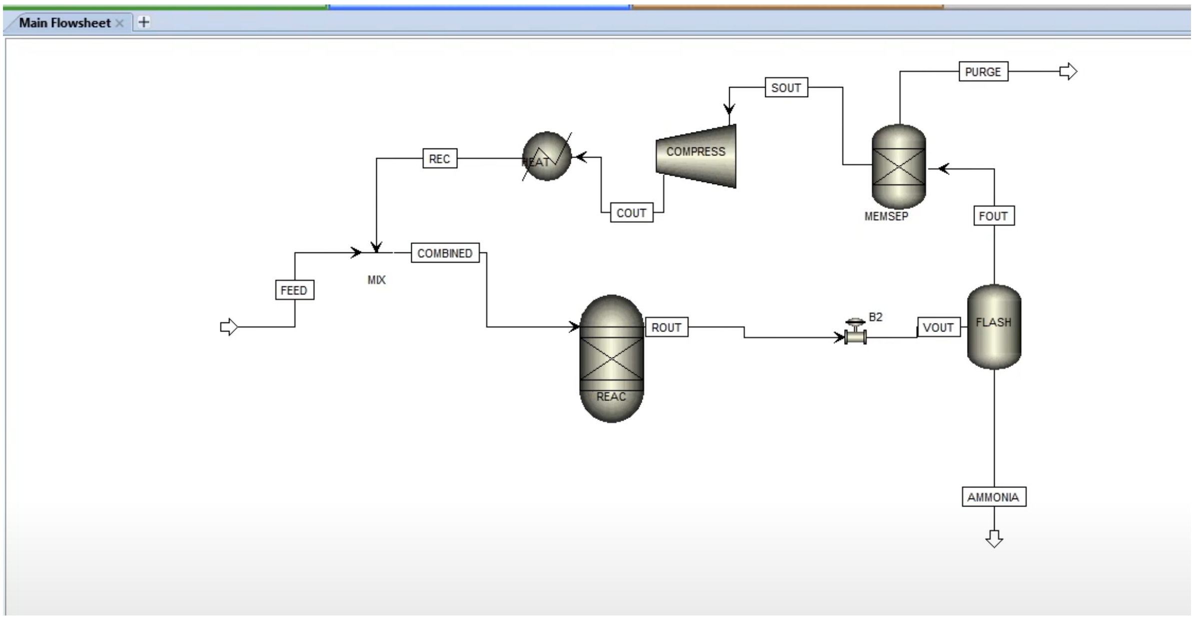

Fig: Complete Flowsheet containing all the required blocks and streams

Now we will used Optimization Tool of Aspen Plus to achieve 99.8% purity of Ammonia.

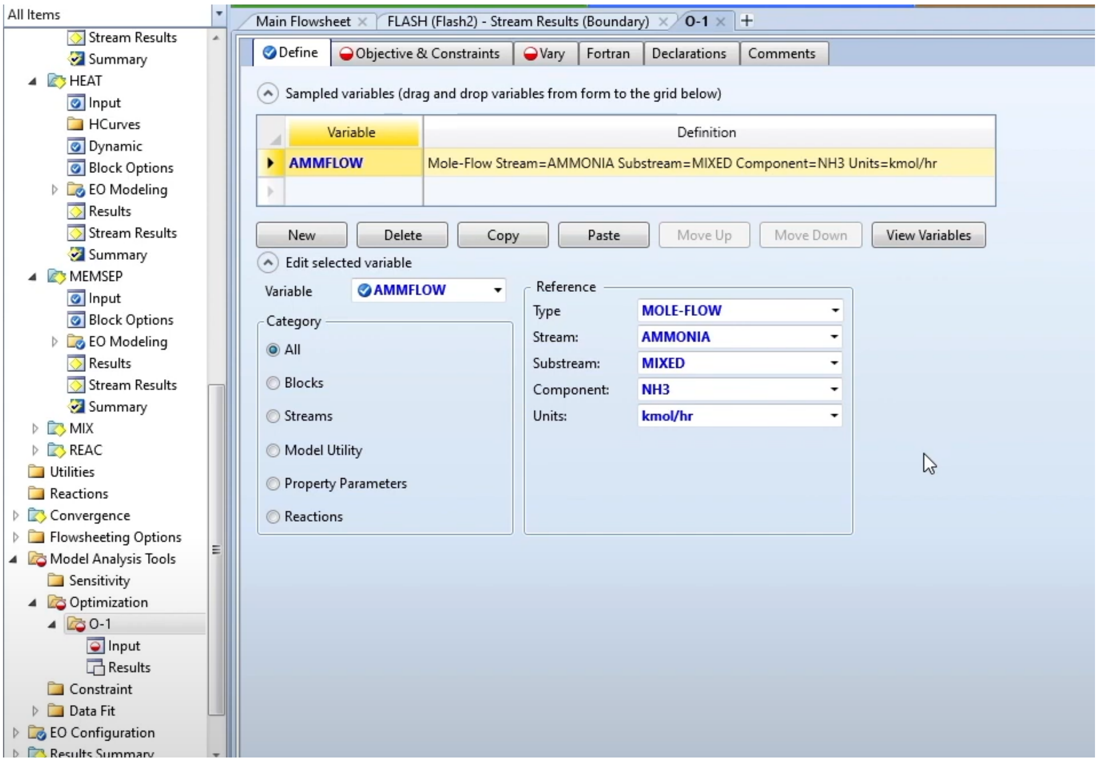

Fig: Defining the variable that will be optimized

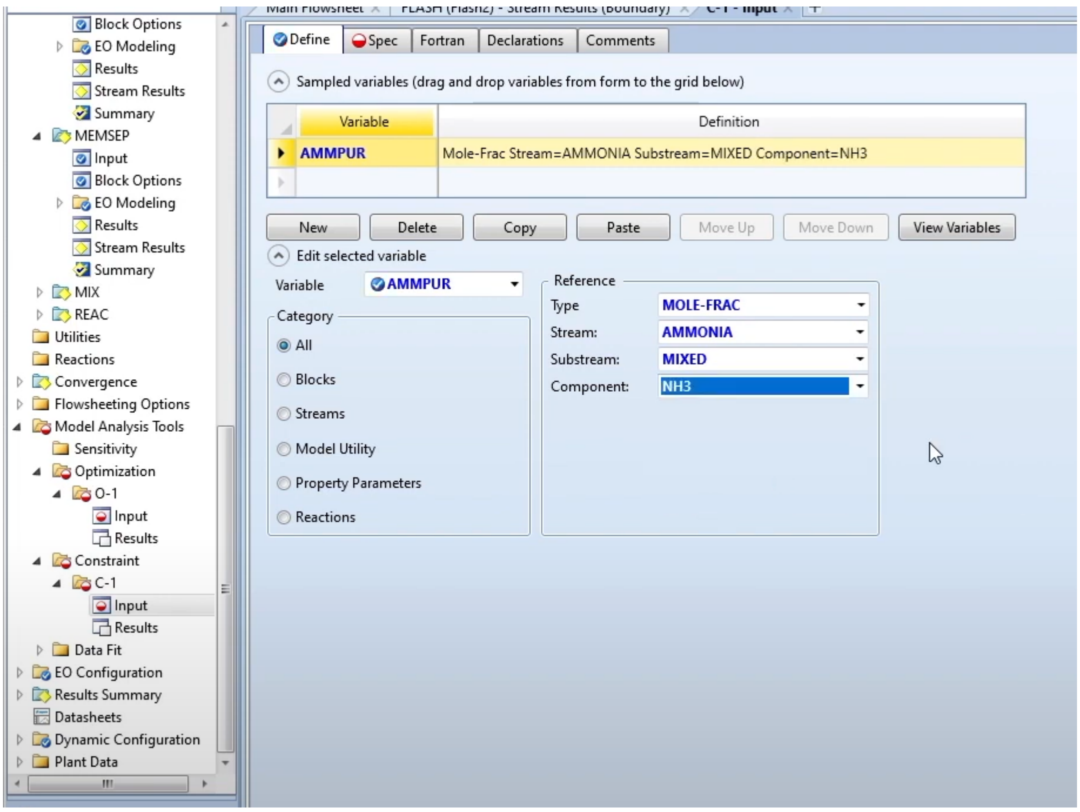

Fig: Defining the constraint

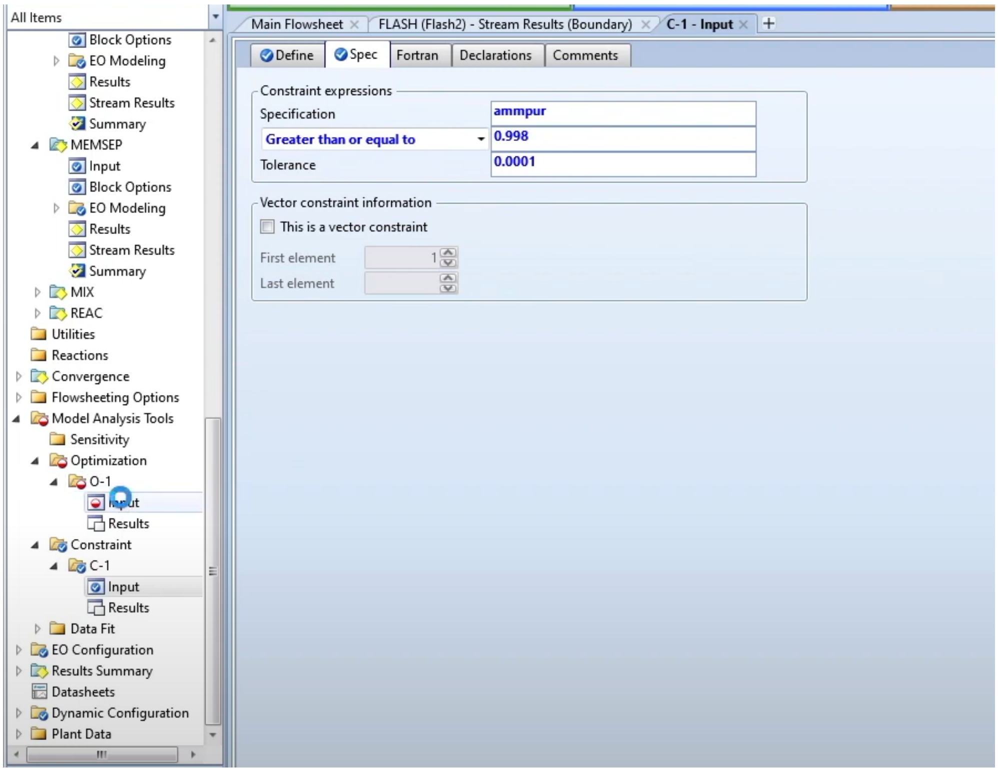

Fig: Setting the Ammonia purity of 99.8%

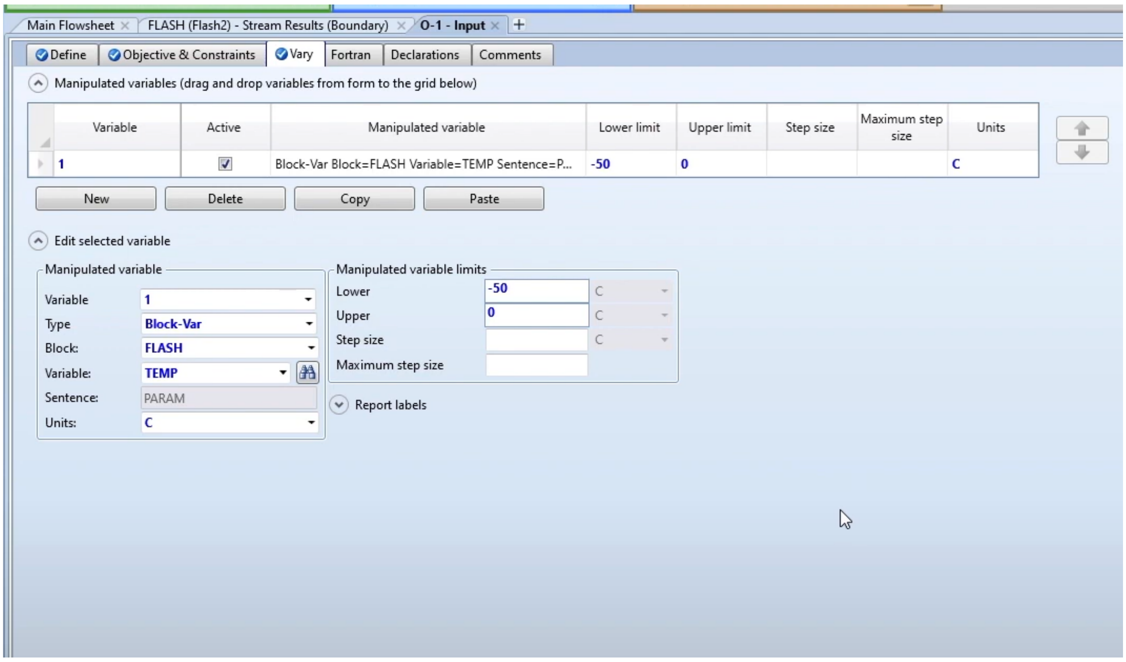

Fig: Defining the variable Flash Temperature

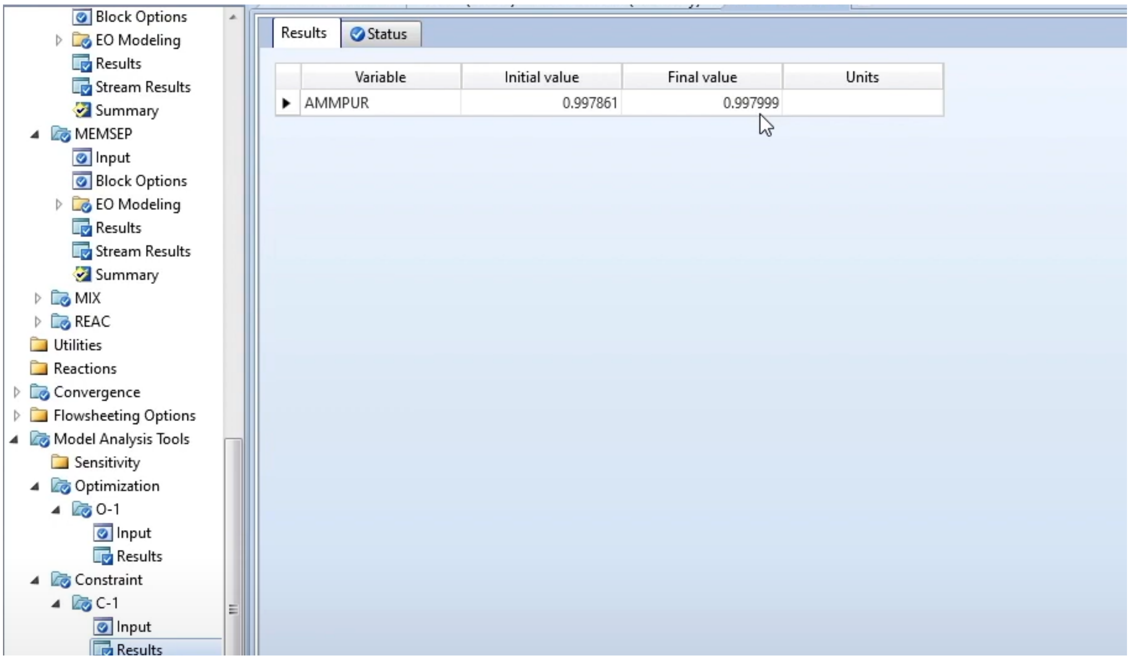

Fig: Results of Varying the Flash Temperature, we achieve 99.7999% purity which is close to desired 99.8%.

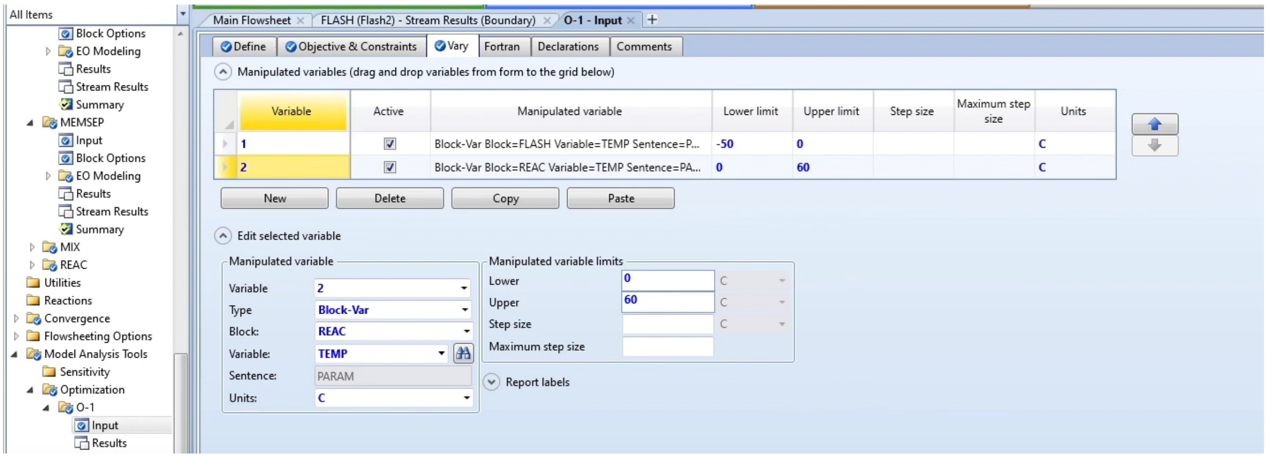

Fig: Defining another variable as Reactor Temperature

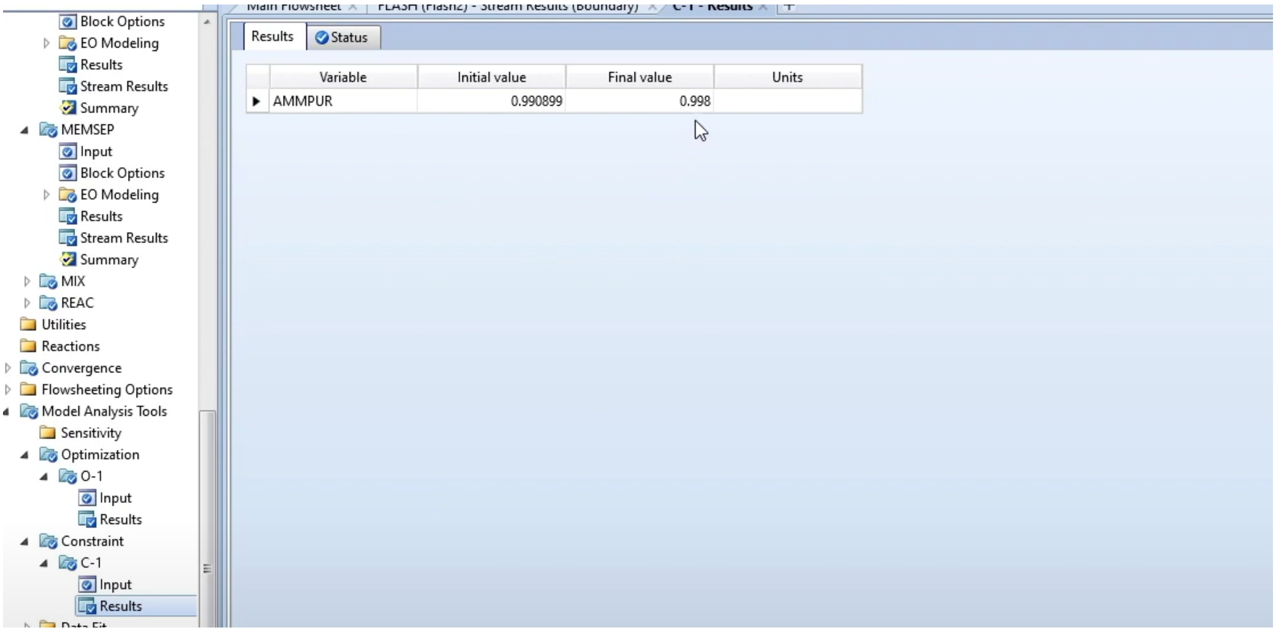

Fig: Results of Varying the Reactor Temperature, we achieve 99.8% purity which is desired.