



PROSIMPLUS APPLICATION EXAMPLE

SIMPLE EXAMPLE

EXAMPLE PURPOSE

The main interest of this simple example is that it allows a progressive approach to process simulation and its main concepts: components involved, thermodynamic models, unit operations and their corresponding operating parameters, recycle loops, etc.

The particular points detailed in this example are the concept of recycling loop and the principles of the simultaneous modular approach used in ProSimPlus.

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CORRESPONDING PROSIMPLUS FILE	<i>PSPS_E01_EN - SimpleExample.pmp3</i>
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Reader is reminded that this use case is only an example and should not be used for other purposes. Although this example is based on actual case it may not be considered as typical nor are the data used always the most accurate available. ProSim shall have no responsibility or liability for damages arising out of or related to the use of the results of calculations based on this example.

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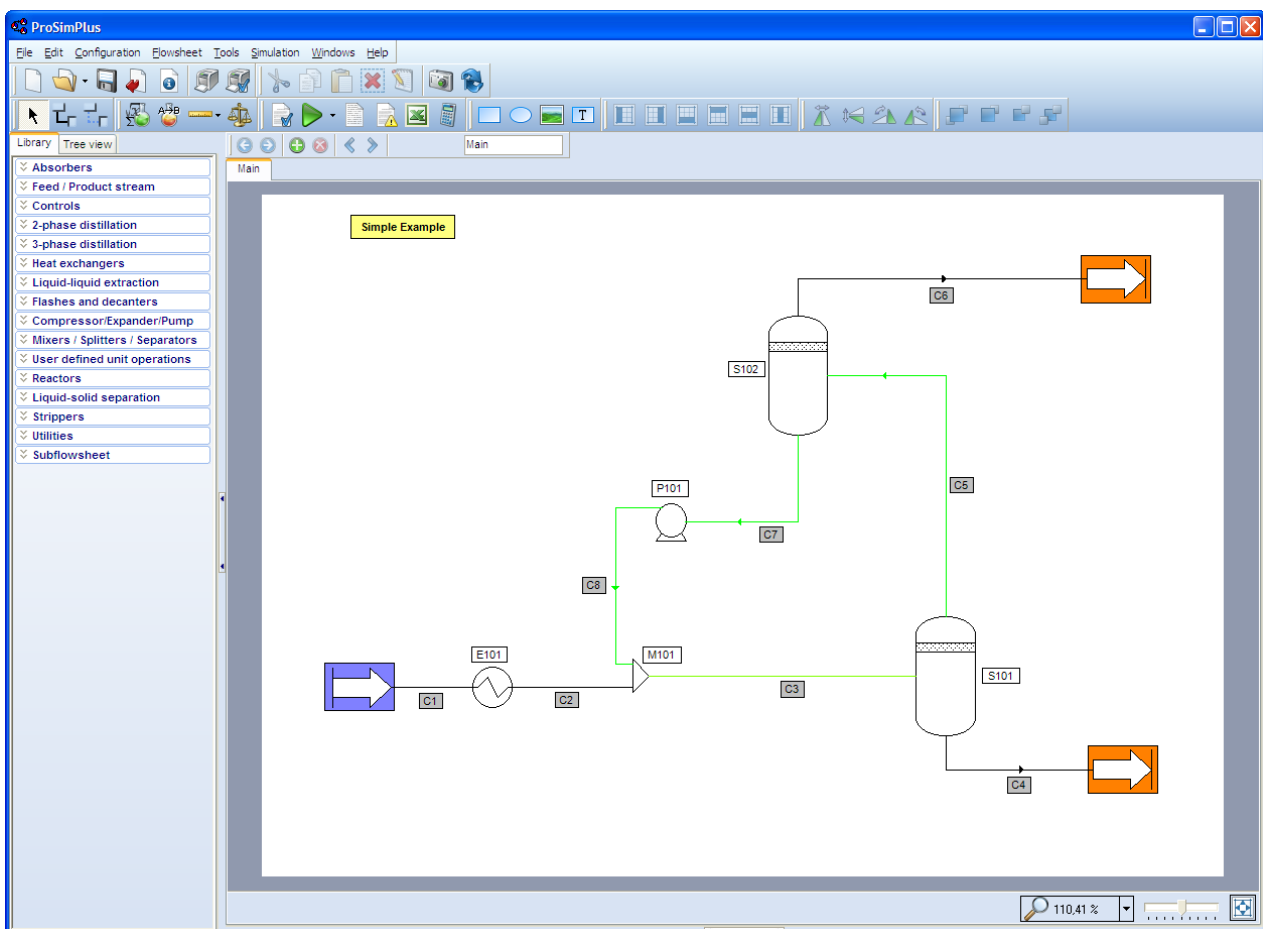
1. PROCESS MODELING

1.1. Process description

This simple example is taken from [1]. In this process, a hydrocarbon mixture is fed (stream C1) and cooled to 15°C (stream C2). It is then mixed with the recycle stream (C8), a pressure drop of 0.3 atm is applied through an expansion valve (not represented), and sent to a flash drum (stream C3 to S101) where liquid and vapor phases are separated. The vapor phase coming out of the drum (stream C5) is sent to a condenser (S102) where it is cooled down to -60°C and expanded to 25 atm. The condensates (stream C7) are fed into a pump (stream C7 to P101) at 75 atm to recycle them at the output of the first heat exchanger. The products are the liquid phase of the flash drum (stream C4) rich in heavy components and the non-condensate phase of the condenser (stream C6) rich in light components.

It has to be noted that for simulation purposes, the expansion valve is simulated together with the phase separation drum in order to reduce the number of modules. It also would have been possible to describe the expansion valve and the separation vessel separately. In fact it is common in process simulation that a physical equipment does not correspond exactly to the simulation model. In a first approach of a process it is frequently preferable to represent the occurring phenomena without taking care of the equipment in which they will be performed in the industrial plant.

1.2. Process flowsheet



Process flowsheet

1.3. Components

Components involved in the simulation are taken from the ProSim standard database, provided with ProSim's software. These components are:

- ❖ Nitrogen
- ❖ Methane
- ❖ Ethane
- ❖ Propane
- ❖ N-Butane
- ❖ N-Pentane
- ❖ N-Hexane
- ❖ N-Heptane
- ❖ N-Octane

1.4. Thermodynamic model

Given the nature of the components in the process (mainly alkanes), the thermodynamic model used to represent phases equilibria and enthalpy calculations is the Soave-Redlich-Kwong (SRK) [2] cubic equation of state, with the binary interaction parameters taken from the database provided with ProSim's software.

1.5. Operating conditions

- ✓ Process feed

	<i>Feed C1</i>
Partial flowrates (kmol/h)	
Nitrogen	9.0
Methane	41.7
Ethane	11.2
Propane	6.2
n-Butane	5.4
n-Pentane	3.0
n-Hexane	8.1
n-Heptane	13.3
n-Octane	2.1
Temperature (°C)	40
Pressure (atm)	75

✓ Heat exchanger E101

<i>Operating parameters</i>	<i>Value</i>
Type	Cooler/Heater
Output temperature (°C)	15

✓ Flash S101

<i>Operating parameters</i>	<i>Value</i>
Type	Liquid-vapor separator
Operating mode	Adiabatic
Pressure drop (atm)	0.3

✓ Flash S102

<i>Operating parameters</i>	<i>Value</i>
Type	Liquid-vapor separator
Operating mode	Fixed temperature and pressure
Output temperature (°C)	-60
Output pressure (atm)	25

✓ Pump P101

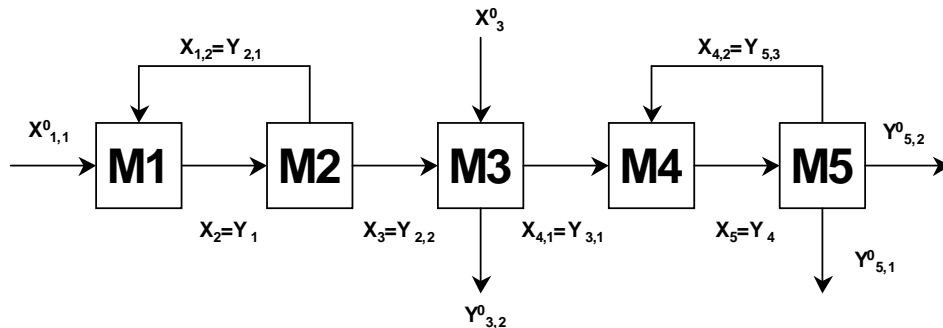
<i>Operating parameters</i>	<i>Value</i>
Output pressure (atm)	75
Volumetric efficiency	65%

1.6. "Hints and Tips"

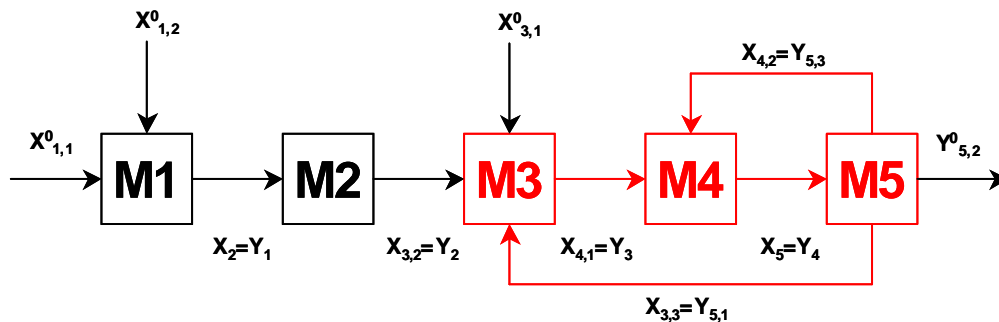
ProSimPlus simulator uses the modular simultaneous approach [3]. This method, derived from the classical "sequential modular approach", carries out the calculation of all equipment of the flowsheet by respecting a calling sequence of the modules. At each module level, knowing the inlet streams and the operating parameters, the module calculates the output streams. This approach is based on a decomposition of the system of equations representing the process. The presence of recycles introduces a difficulty in the generation of this sequence of calculation.

The diagram of simulation represents an oriented graph in which each node corresponds to a module and each arc to all the variables of a stream. The orientation of arcs is defined by the flow direction of information in the diagram. The traditional techniques for the decomposition of the sparse systems can then directly apply to such graphs and

make it possible to highlight the subsystems which cannot be broken up directly (called maximum cyclic networks). A maximum cyclic network (MCN) is defined as a set of modules connected by streams and forming one (or several) cycle(s) not included in another cycle. Two examples of graphs and corresponding MCNs are presented hereafter.



Example with 2 MCNs: (M1, M2) and (M4, M5)



Example with 1 MCN: (M3, M4, M5)

MCNs can then be solved sequentially, each ones after the others according to an order which follows the direction of circulation of flows.

It should be noted that for the same graph, there are multiple solutions and that the choice of a set of “tear streams” generally relies on heuristic rules. Finally, a sequence of calculation is generated for the set of “tear streams” selected.

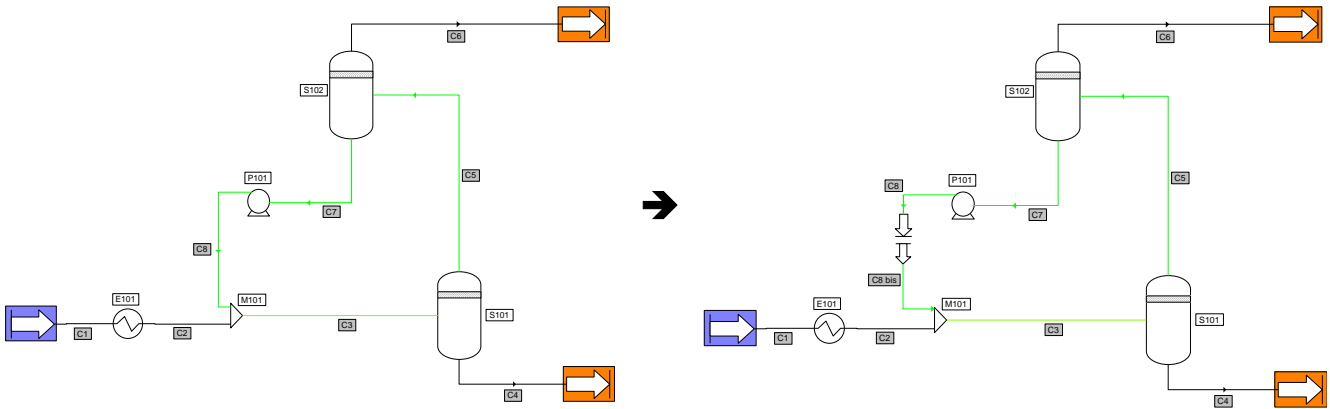
In the second example presented above, the sequence of calculation associated with the tear stream $X_{4,2}$ and $X_{3,3}$ is as follows: M1, M2, (M3, M4, M5). The choice of X_5 as the tear stream led in this case to the sequence: M1, M2, (M5, M3, M4). Brackets were used to frame MCNs because each MCN requires the implementation of an iterative process to reach convergence.

The examples presented here are sufficiently simple so that one can easily determine MCNs, the “tear streams” and list of calculation of the modules. Obviously it is not the same for more complex flowsheets which contain many strongly inter-connected modules. Specific algorithms are used in ProSimPlus to achieve these various tasks.

In short and on the numerical level, the resolution of a problem of pure simulation according to the simultaneous modular approach leads to three levels of calculation:

- the property server level, such as for example the solution of an equation of state;
- the module level: each model of unit is solved separately within a module according to a numerical approach adapted to the system of equations implemented;
- the flowsheet level: where the equations associated with the streams with recycling are solved.

In our current example, ProSimPlus the stream C8 as the tear stream. One can schematize the approach adopted by the simulator for the resolution as follow:



Flowsheet as shown

Flowsheet actually solved by ProSimPlus

It should be noted that the user can easily modify the numerical parameters of the Constraints/Recycles manager which ensures the convergence of the simulation. To achieve this, the user must use a module of the type "Constraints and Recycles" that he simply drops on the process flowsheet and does not have to connect to any of the modules.



2. RESULTS

2.1. Comments on results

The calculation sequence (the order of calculation of the modules) is generated automatically. At the recycle level, no stream is initialized and ProSimPlus chooses to make the C8 stream converge.

The convergence of the recycle is obtained in 3 iterations.

2.2. Mass and energy balances

In this example, the mass and energy balances are presented in one of the many forms available within ProSimPlus. The user has the choice to display all or part of results obtained and to present them in the selected units and in the selected form. He can in particular decide to display results in the form of mass or molar flowrates, of mass or molar fractions and total flowrates. He can also select the properties which will appear at the results level. It is the case for the HTML results file, but also for the "summary table" which appears at the bottom of the flowsheet and which can be directly exported to other applications.

Streams		C1	C2	C3	C4
From		FEED	E101	M101	S102
To		E101	M101	S102	Process outlet (heavy)
Partial flows		kg/h	kg/h	kg/h	kg/h
NITROGEN		252,121698	252,121698	253,025015	47,7441733
METHANE		668,984765	668,984765	678,071323	256,195079
ETHANE		336,779523	336,779523	359,529881	259,174311
PROPANE		273,398523	273,398523	298,029453	260,015346
n-BUTANE		313,866595	313,866595	329,249317	312,514551
n-PENTANE		216,451046	216,451046	221,139957	216,366317
n-HEXANE		698,035843	698,035843	703,582226	698,023934
n-HEPTANE		1332,71321	1332,71321	1337,27118	1332,71103
n-OCTANE		239,88533	239,88533	240,23728	239,885296
Total flow	kg/h	4332,23653	4332,23653	4420,13564	3622,63004
Total flow	m3/h	19,384102	16,5970197	16,6311488	6,48038042
Physical state		Liq./Vap.	Liq./Vap.	Liq./Vap.	Liquid
Temperature	°C	40	15	13,5077605	13,4680112
Pressure	atm	74,9999797	74,9999797	74,9999797	74,6999798
Enthalpy	kcal/h	-263645,747	-332858,996	-344466,136	-325728,507

Streams		C5	C6	C7	C8
From		S102	S102	S102	P101
To		S102	Process outlet (lights)	P101	M101
Partial flows		kg/h	kg/h	kg/h	kg/h
NITROGEN		205,280842	204,377525	0,90331681	0,90331682
METHANE		421,876244	412,789685	9,08655885	9,08655776
ETHANE		100,35557	77,6051934	22,7503764	22,7503584
PROPANE		38,0141072	13,3831946	24,6309126	24,6309307
n-BUTANE		16,7347661	1,35205986	15,3827062	15,3827216
n-PENTANE		4,77364021	0,08471982	4,68892039	4,68891134
n-HEXANE		5,55829203	0,01189465	5,54639738	5,54638358
n-HEPTANE		4,56015351	0,00216851	4,55798501	4,55797275
n-OCTANE		0,35198412	3,3672E-05	0,35195045	0,35194943
Total flow	kg/h	797,505599	709,606474	87,8991241	87,8991024
Total flow	m3/h	10,21336	21,5629081	0,1613734	0,16094906
Physical state		Vapor	Vapor	Liquid	Liquid
Temperature	°C	13,4680112	-60	-60	-55,9900484
Pressure	atm	74,6999798	24,9999932	24,9999932	74,9999797
Enthalpy	kcal/h	-18737,6481	-32244,126	-11907,9562	-11607,337

3. REFERENCES

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