Comparison of Chemical Process Simulators: Aspen vs. HYSYS

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Abstract

Since 2007, Aspentech provides to universities, a single closed software package, joining two process simulators: Aspen Plus/Dynamics and HYSYS. This work provides a comparison, analysing the integration between them and other products included into the software package.

As a case study, it was selected “Ammonia Converter Design”, with available tutorials for both Aspen Plus and HYSYS, from multimedia CD “Using Process Simulators in Chemical Engineering” by Seider, Seader & Lewin. Each of these steady-state simulations has its own thermodynamic model and specific database. Using, for reference, an ammonia synthesis process published on “Ullmann's encyclopedia of industrial chemistry”, it has been realized that none of the thermodynamic models simulate accurately the ammonia condensation. A new Aspen Plus thermodynamic model, published by AspenTech in April/2008, provided good agreement with the reference. But only the next version (V7.0) will allow the implementation of the same thermodynamic model over HYSYS.

To run a dynamic simulation, HYSYS *Dynamics Assistant* helps to make the initial spec of the model. Instead, Aspen Plus *Pressure Checker* only pin-points problems, that must be all resolved by the user. Time factors (simulation time)/(real-time) for the dynamic simulations are resumed in the following table:

Update frequency	**Simulation time/Real-time**	
	HYSYS	**Aspen Dynamics**
1 min^{-1}	**6,0**	**93,9**
1 s^{-1}	**4,5**	**2,2**

HYSYS does not simulate processes involving polymers and it is more limited than Aspen Plus/Dynamics, for solid operations or reactive distillation. For other cases, HYSYS is more adequate.

Introduction

Since 1997 Aspen Plus steady-state process simulator is adopted at Instituto Superior Técnico for Chemical Engineering curriculum. The first version available for students was Aspen 9, running over Microsoft DOS 6.2. First in-house contact with HYSYS was provided by an Hyprotech presentation, in 1998. HYSYS impressed the students at the time, with the appealing interface of a dynamic simulation. Competitive solution from AspenTech, Aspen Dynamics was locally available right after. But the lack of in-house expertise, a cumbersome steady-state to dynamic migration process and a very different user interface between Aspen Plus and Dynamics resulted in the stamp “too difficult to use”.

Dynamic simulation was still lectured, recurring to Matlab Simulink and GPROMS, but it was still missing the ability to pick a plantwide steady-state simulation and get into a *dynamic* plantwide simulation. As a 5th year student working in plant design with Aspen Plus steady state simulator, I was worried with startup and shutdown procedures, wondering if the plant would be able to reach the desired “steady state”, from the sketched Pipe & Instrumentation Diagrams.

In 2002 HYSYS got into Aspentech’s portfolio, but still available to universities as a competitive option, against Aspen Plus/Dynamics. At Instituto Superior Técnico we sticked with Aspen Plus/Dynamics. Only in 2007 HYSYS arrived to us, thanks to the new Aspentech software package policy for universities: one (big) closed package for everyone, no option features available.

Working with Aspentech software

The full software portfolio is published in http://www.aspentech.com/products, but for universities, the available subset is http://www.aspentech.com/corporate/university/products.cfm. You should check with your local Aspentech contact person, searching for the local upgrade schedule. Your school can be up to a year behind the latest software release.

You should have access to the product documentation. At least since 2004, a documentation disk is included in the Aspentech disk bundle. The documentation disk can be installed or browsed through the included DVDbrowser.exe. This application displays on the default web browser, both PDF manuals and program-context help files.

Forgiving the aging of Aspen Plus 11, HYSYS 3.01 or MATLAB 5.3 (® MathWorks), the Multimedia CD "Product and Process Design Principles: Synthesis, Analysis, and Evaluation" is the right start tool to learn how to use these programs. This Multimedia CD is included in the book "Product and Process Design Principles: Synthesis, Analysis, and Evaluation", by Seider, Seader & Lewin [1]. An important upgrade is offered by these authors in the website http://www.seas.upenn.edu/~dlewin/Upgrade_2004.htm.

For process case studies over Aspentech software, these sources should be considered:

I) "Plantwide Dynamic Simulators in Chemical Processing and Control" [2]. Whenever possible, each case is implemented in both Aspen Plus/Dynamics (version 10.2.2) and HYSYS (version 2.4.1). Having the dynamic simulation as objective, the reaction kinetics is supplied, but kinetic data is decided in some cases. Luyben does not have a commitment to use the same data bases and models of physical properties in the two simulators. The differences and difficulties felt in the implementation of each case are highlighted, in each one of the simulators.

II) Aspen PEP. Is the implementation of Process Economics Program reports from the SRI Consulting, over Aspen Plus. The product was discontinued, having the last developments occurred in version 11.1. The models are strictly for steady state. It was verified that some models do not converge, even in the original version of the program.

Aspen and HYSYS provide a set of examples and some of them are detailed as tutorials, in the documentation. More examples can be found at http://support.aspentech.com, through your local support person. It is not likely to have useful input from Aspentech user forums: there are few academic participants and Aspentech consultants are only helpful for enterprise users.

For the development of this paper, the interesting cases are those with available kinetics, implemented on Aspen Plus, but not necessarily on HYSYS. The ammonia synthesis was chosen, for being a well known process. Specifically, it is adopted the implementation from the Multimedia CD [1], the tutorial of "Amonnia Converter Design". It is provided, in this CD, the steady state files for both programs: Aspen Plus and HYSYS.

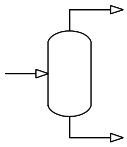
As described in the CD, this case includes three plug-flow adiabatic reactors, in series, with addition of reagents to the 2nd and the 3rd reactors. There is a heat exchanger with the exit from the 3rd reactor and the feed to the 1st reactor. The global rea"ctor conversion is maximized, manipulating the fresh-feed flows to the 2nd and 3rd reactors: Aspen Plus has a "design spec" and HYSYS has an "optimizer".

Through the present work, the case will be complemented with the separation of ammonia and recycling of reagents, illustrating the different way as recycle is implemented, in the two simulators.

Physical Property models

To compare the two process simulators, they should share the same thermodynamic model. That is not the case, with the simulations provided from the Multimedia CD [1]. In Aspen Plus file is applied Predictive Soave-Redlich-Kwong equation of state; in HYSYS is applied Soave-Redlich-Kwong equation of state. Furthermore, none of these thermodynamic models provides good accuracy for ammonia condensation. To check it, an ammonia synthesis process from "Ullmann's encyclopedia of industrial chemistry" [3] is used as reference. There are two ammonia condensate separators, operating around 300 bars, with temperatures of 20ºC and -1ºC. The next figure compare the results obtained on Aspen Plus and HYSYS, applying the respective thermodynamic models as defined on Multimedia CD [1]. Aspen Plus simulation is bad, HYSYS is not good enough.

	Ullmann's	Aspen	HYSYS
H_2	**55,73%**	51,47%	54,36%
N_2	**19,43%**	18,80%	19,84%
NH_3	**5,55%**	12,05%	6,84%
Ar	**5,20%**	4,81%	5,06%
CH_4	**14,09%**	12,87%	13,90%

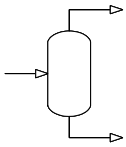


30,0 MPa

20ºC

	Ullmann's	Aspen	HYSYS
H_2	**1,05%**	3,48%	1,04%
N_2	**0,40%**	1,29%	0,53%
NH_3	**97,34%**	84,88%	95,17%
Ar	**0,18%**	0,38%	0,23%
CH_4	**1,03%**	9,97%	3,03%

	Ullmann's	Aspen	HYSYS
H_2	**61,21%**	60,30%	60,83%
N_2	**21,07%**	20,75%	20,93%
NH_3	**2,72%**	4,17%	3,35%
Ar	**4,03%**	3,97%	4,00%
CH_4	**10,97%**	10,81%	10,89%



31,7 MPa

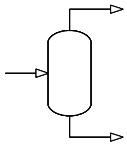
-1ºC

	Ullmann's	Aspen	HYSYS
H_2	**0,82%**	No liquid	0,72%
N_2	**0,28%**		0,34%
NH_3	**98,20%**		96,75%
Ar	**0,10%**		0,12%
CH_4	**0,60%**		2,08%

Figure 1: The original physical property models from Multimedia CD are not valid for ammonia condensation (PSRK for Aspen Plus and SRK for HYSYS).

A better thermodynamic model is available from http://support.aspentech.com. There is a case study of ammonia synthesis from natural gas over Aspen Plus, published on April/2008. It uses Redlich-Soave-Kwong equation of state with Boston-Mathias alpha function. It is supplied a set of binary parameters between ammonia and each of the other components; and three ammonia thermodynamic parameters within the "pure" databank are changed. These changes (binary parameters and the 3 "pure" ammonia parameters) also improve HYSYS Soave-Redlich-Kwong model, as shown by the following results:

	Ullmann's	Aspen	HYSYS
H_2	**55,73%**	54,29%	54,58%
N_2	**19,43%**	19,83%	19,91%
NH_3	**5,55%**	6,67%	6,23%
Ar	**5,20%**	5,06%	5,09%
CH_4	**14,09%**	14,14%	14,19%

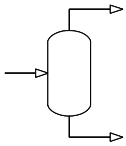


30,0 MPa

20ºC

	Ullmann's	Aspen	HYSYS
H_2	**1,05%**	1,18%	1,09%
N_2	**0,40%**	0,46%	0,54%
NH_3	**97,34%**	97,19%	97,04%
Ar	**0,18%**	0,18%	0,20%
CH_4	**1,03%**	0,98%	1,12%

	Ullmann's	Aspen	HYSYS
H_2	**61,21%**	60,83%	61,01%
N_2	**21,07%**	20,93%	20,99%
NH_3	**2,72%**	3,33%	3,05%
Ar	**4,03%**	4,00%	4,02%
CH_4	**10,97%**	10,90%	10,93%



31,7 MPa

-1ºC

	Ullmann's	Aspen	HYSYS
H_2	**0,82%**	0,82%	0,77%
N_2	**0,28%**	0,30%	0,36%
NH_3	**98,20%**	98,22%	98,12%
Ar	**0,10%**	0,10%	0,11%
CH_4	**0,60%**	0,55%	0,64%

Figure 2: Both property models provide good agreement with the Ullmann's reference. Aspen Plus uses RKS-BM, as proposed by Aspentech. HYSYS uses SRK, but with the databank changes proposed by Aspentech [4].

The following figures show the changes to Aspen Plus databanks, from Aspentech's Apr/2008 Ammonia Model [4]. The equivalent changes have been applied over HYSYS (not shown).

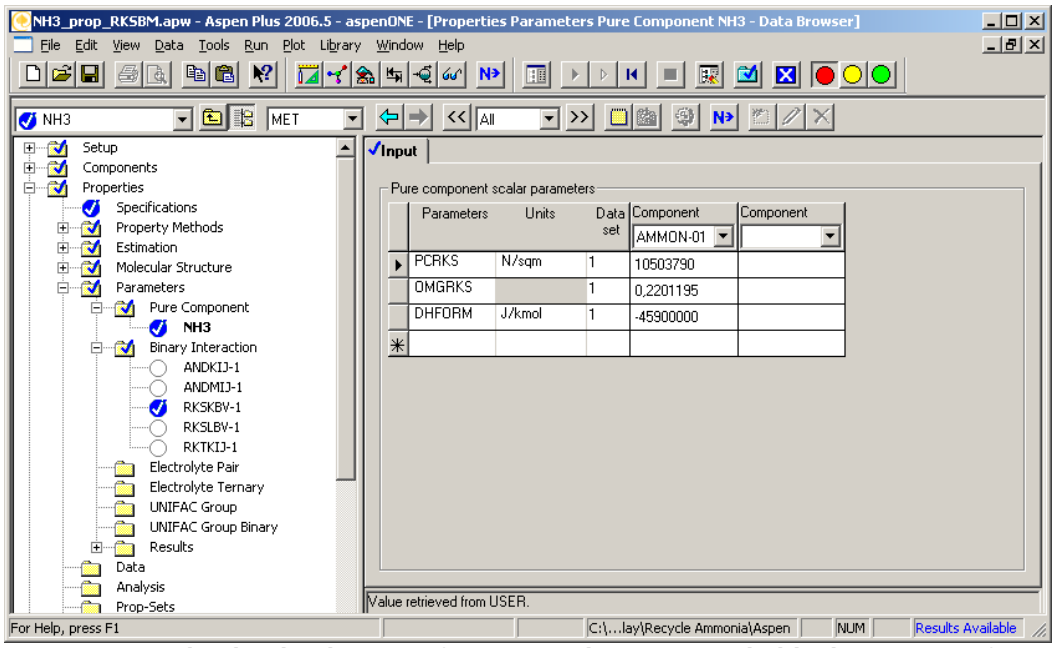


Figure 3: Pure databank changes for ammonia. PCRKS (critical pressure for RKS equation of state) and DHFORM (formation enthalpy) are similarly described over HYSYS. OMGRKS (omega factor for RKS equation of state) is the SRK Acentricity on HYSYS.

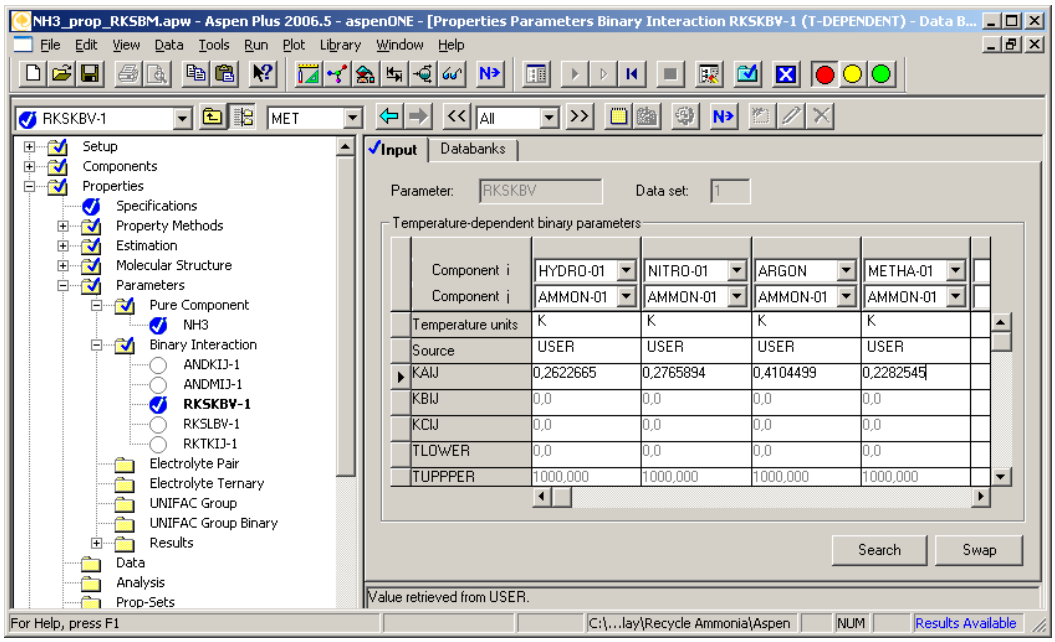


Figure 4: Ammonia binary interaction parameters, as proposed by Aspentech. RKSKBV (Redlich-Kwong-Soave "K_{ij} Binary Values") are symmetric parameters: the value from "i" to "j" is the same from "j" to "i".

On HYSYS 2006.5, "Aspen Properties" is listed as physical property model, providing the same equations of state available for Aspen Plus, but not the same databanks. Next HYSYS V7.0 will overcome this limitation [4].

Steady State simulations

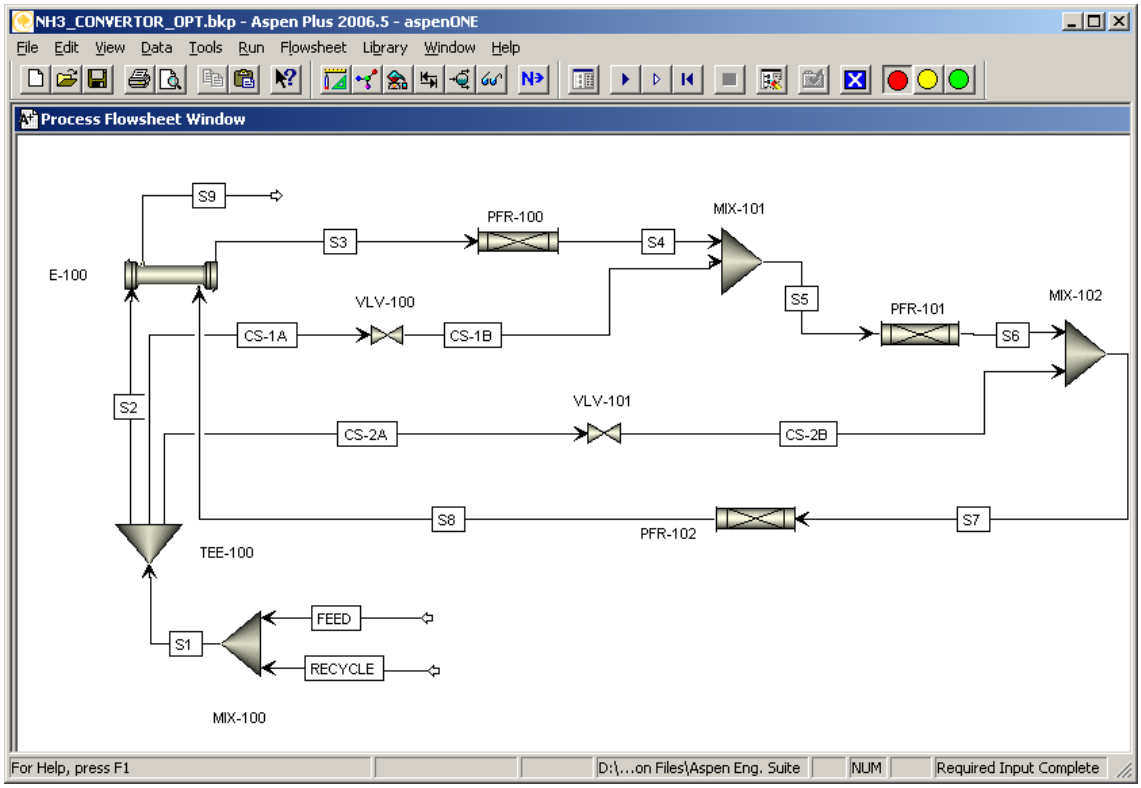


Figure 5: Aspen Plus simulation, as provided from Multimedia CD [1].

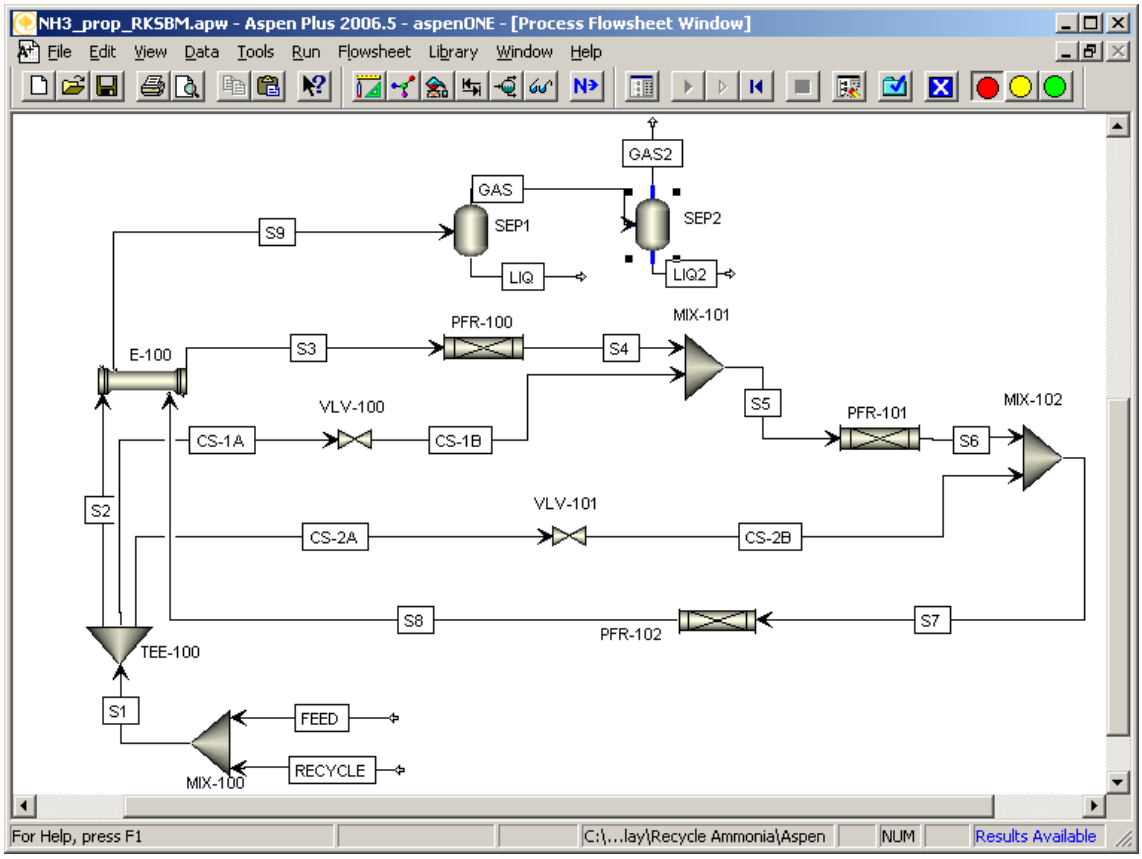


Figure 6: Aspen Plus simulation, with added isothermal gas-liquid separators, acting as ammonia condensers. SEP1 operates at 25ºC. SEP2 temperature is chosen to provide 0,015 ammonia molar fraction on GAS2, which is the value specified on RECYCLE.

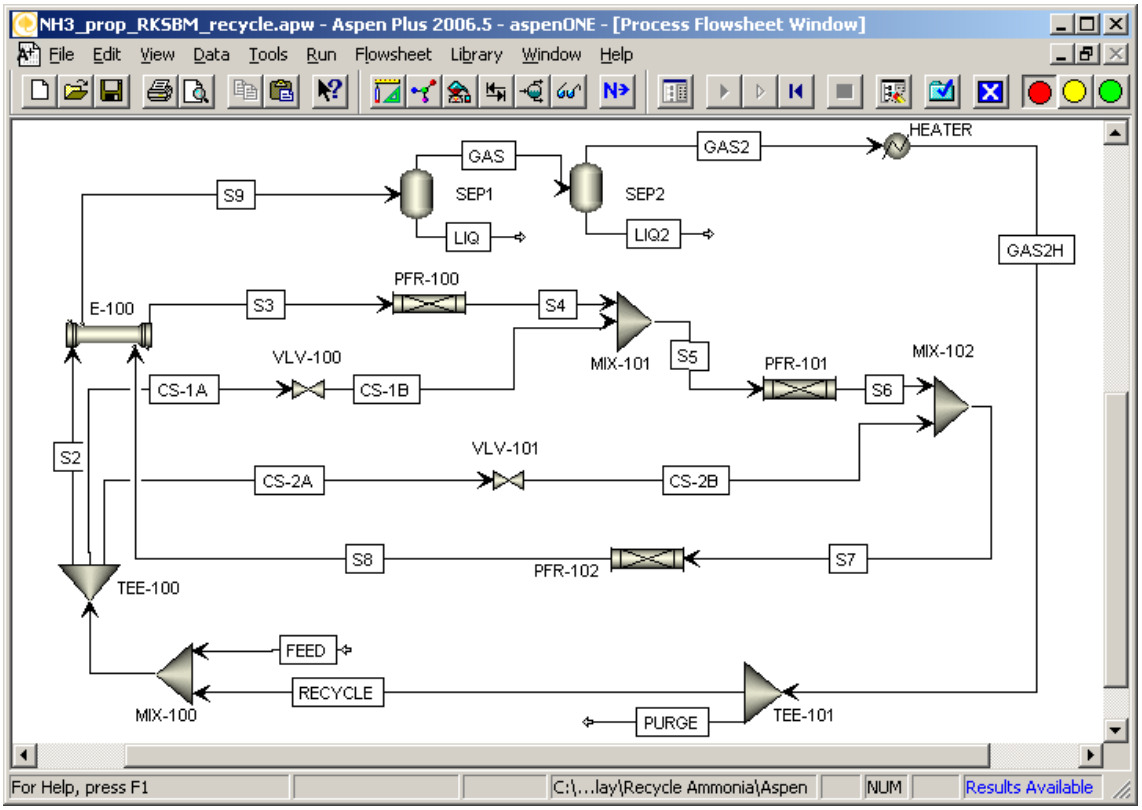


Figure 7: Recycle loop on Aspen Plus.

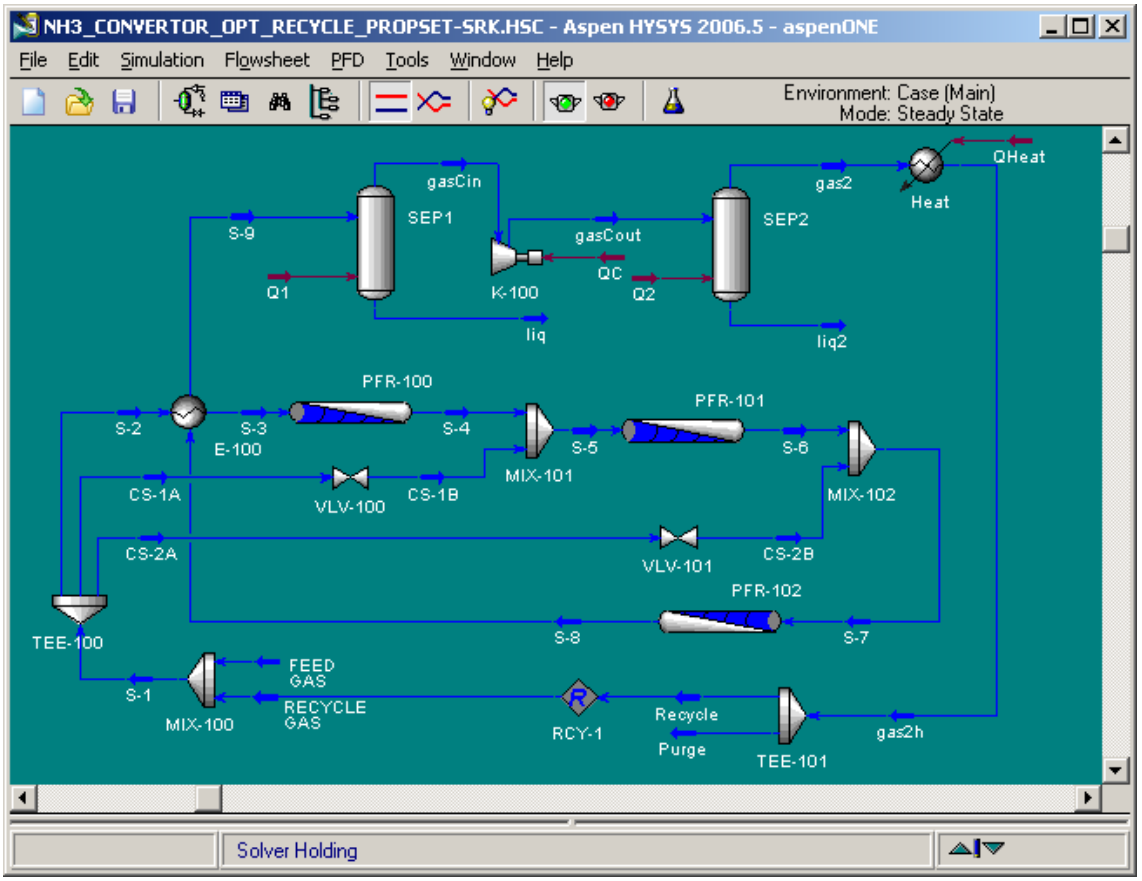


Figure 8: Recycle loop on HYSYS.

Dynamic simulations

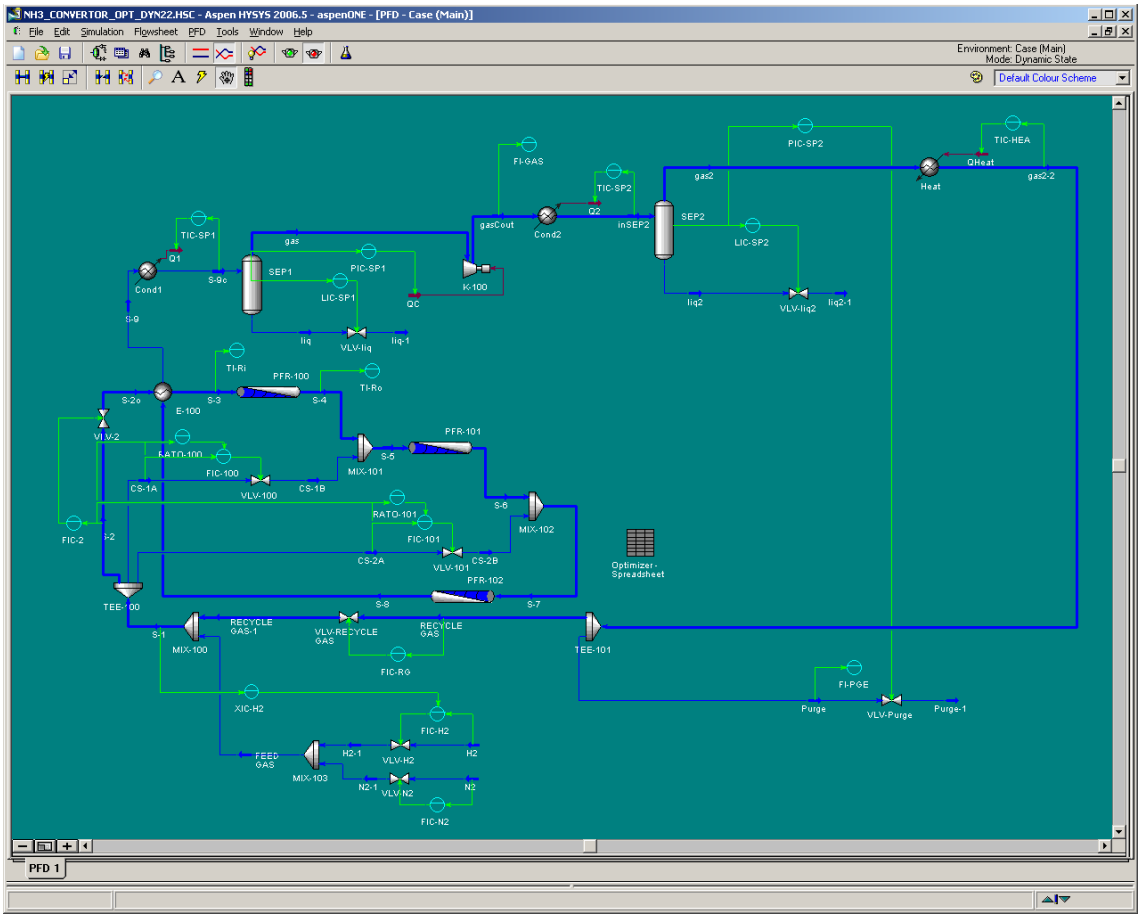


Figure 9: HYSYS "Pipe & Instrumentation Diagram"

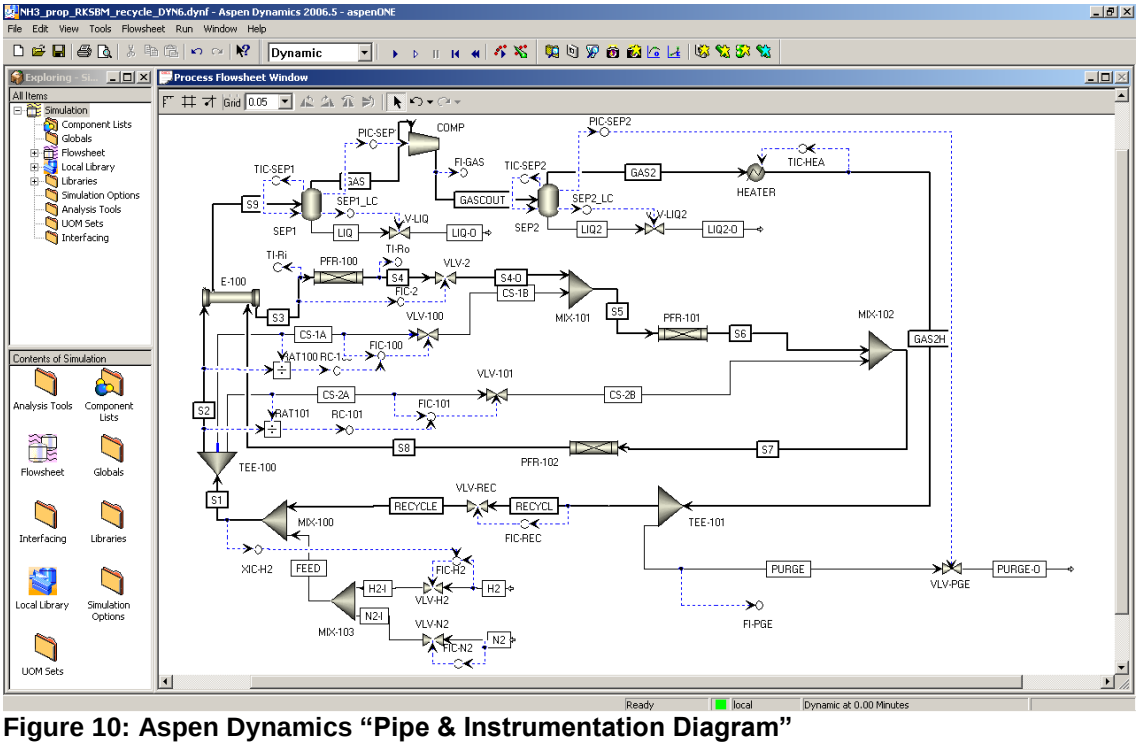


Figure 10: Aspen Dynamics "Pipe & Instrumentation Diagram"

Conclusion

Given the experience collected from published cases [1], [2], Aspentech support site [4] and program-included examples, it is suggested the selection between Aspen Plus/Dynamics and HYSYS, given the problem to solve. If both programs are suitable, the first option is the preferred one.

Does the problem include:

1) **Polymers**?
   a) Polymerization reaction: **Aspen Plus**
   b) Separation between polymer fractions: **Aspen Plus**
   c) Separation based on solvent polymer solubility: **Aspen Plus**
   d) Solid separation: **See 2).** *Hypocomponent*-HYSYS; *Pseudocomponent*-Aspen Plus.
   e) With dynamic simulation: **Aspen Plus/Dynamics.**
2) **Solids**? Solid operations are not available for dynamic simulation.
   a) Cyclone: **HYSYS** or Aspen Plus
   b) Hydrocyclone: **HYSYS** or Aspen Plus
   c) Vacuum rotary filter: **HYSYS** or Aspen Plus
   d) Baghouse filter: **HYSYS** or Aspen Plus
   e) Other solid-phase operation: check the availability on **Aspen Plus**.
3) **Reactive distillation**?
   a) Steady state only: **Aspen Plus** or HYSYS
   b) Dynamic simulation: **Aspen Plus/Dynamics.** For HYSYS, Aspentech support [4] does not provide information. Luyben has reported failure [2].
4) **Dynamic** simulation?
   a) Dynamic simulation to preview an upset result, hours after it has occurred: **Aspen Plus/Dynamics** or HYSYS
   b) Dynamic simulation, focused on controller tuning, testing different tuning methods: **Aspen Plus/Dynamics** or HYSYS
   c) Dynamic simulation to check if implemented control loops allow starting up and/or shutdown the process: **HYSYS** or Aspen Plus/Dynamics.

Aspen Plus/Dynamics is capable to solve more problems than HYSYS. But excluded the particular problems, indicated above, HYSYS should be preferred, because:
1) In steady state, the bidirectional calculation makes possible to resolve the problem, supplying the data of exit streams and without set up design-specs (restrictions and convergence objectives of the simulation);
2) Active solver, that produces resulted (or errors), as soon as the enough information is supplied;
3) Still in steady state, it allows to add control loops to the flowsheet;
4) Dynamic Assistant, that facilitates so much the migration for dynamic simulation;
5) Common interface, between steady state and dynamic simulation;
6) One single file for each simulation.

References

[1] Multimedia CD “Using Process Simulators in Chemical Engineering”, offered with the book “Product and Process Design Principles: Synthesis, Analysis, and Evaluation”, 2nd Edition, Seider, Seader & Lewin
© 2004 John Wiley & Sons, Ltd., ISBN: 978-0-471-21663-6

[2] “Plantwide Dynamic Simulators in Chemical Processing and Control”, 1st edition, Luyben
© 2002 CRC Press, ISBN: 978-0824708016

[3] “Ullmann's encyclopedia of industrial chemistry”, 5th ed., Volume A2, page 201
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[4] http://support.aspentech.com