

From: [Antonio Brandão](#)
To: [Sigurd Skogestad](#)
Subject: Re: Letter to Editor - <https://doi.org/10.1016/j.compchemeng.2008.03.001>
Date: onsdag 13. mars 2024 15:04:24
Attachments: [image001.png](#)
[image002.png](#)
[image003.png](#)
[responseToLetterToEditor.docx](#)

Hello Sigurd.

Here goes the information.

Hope this helps.

Best regards.

Antonio

On Thu, Mar 7, 2024 at 12:16 PM Antonio Brandão <brandao@eq.ufcg.edu.br> wrote:

No reaction or little reaction?

Very little, almost nothing.

I still don't understand. I guess you want to use the same k as Morud. How do you get this?

Morud divided by rho and got high conversions at P = 200bar and Ti = 415C, but dividing k by rho in Aspen leads to no reaction:

```
k1=1.79e+4*exp(-87090/(R*(T+273)));  
k2=2.57e+16*exp(-198464/(R*(T+273)));  
pnh3=x*p ; % partial pressure (bar)  
pn=(1-x)*0.25*p;  
ph=(1-x)*0.75*p;  
r=k1*pn*ph^1.5/pnh3 - k2*pnh3/ph^1.5; % [mol N2/ m3 cat, h]  
r=r*34/rho/3600;
```

Anyway, what would you suggest doing if you should redo the paper?

For now, it is exactly redoing the paper... Frankly, I think whatever comes out the same CVs will be selected in both modes. Maybe dynamics will change a bit...

Morud's has always been the benchmark. To try to be more convincing and avoid high conversion at the first few centimeters, my guess is that the factor f must be adjusted from the original 4.75 to fit Morud's. For that to happen, Morud's conditions must be replicated in Aspen and f adjusted accordingly, and then hope to get similar mass and energy balances, plantwide results, and dynamic behavior. This is too much work, and right now I'm very (extremely) busy.

On Thu, Mar 7, 2024 at 11:50 AM Sigurd Skogestad <sigurd.skogestad@ntnu.no> wrote:

No reaction or little reaction?

Anyway, what would you suggest doing if you should redo the paper?

I still don't understand. I guess you want to use the same k as Morud. How do you get this?

-Sigurd

From: Antonio Brandão <brandao@eq.ufcg.edu.br>
Sent: Thursday, March 7, 2024 3:19 PM
To: Sigurd Skogestad <sigurd.skogestad@ntnu.no>
Subject: Re: Letter to Editor - <https://doi.org/10.1016/j.compchemeng.2008.03.001>

Hello.

I used his k, not ours to simulate.

Maybe this figure is more clear (streams 3 and 4 are feed and product of bed 1, and so forth):

	Units	3	4	28	6	29	8
Temperature	C	231.92	232.042	231.994	232.138	232.089	232.283
Pressure	bar	200.194	199.194	199.094	198.094	197.994	196.994
Molar Vapor Fraction		1	1	1	1	1	1
Molar Liquid Fraction		0	0	0	0	0	0
Molar Solid Fraction		0	0	0	0	0	0
Mass Vapor Fraction		1	1	1	1	1	1
Mass Liquid Fraction		0	0	0	0	0	0
Mass Solid Fraction		0	0	0	0	0	0
Molar Enthalpy	kcal/mol	-0.560186	-0.560226	-0.560462	-0.560509	-0.560662	-0.560727
Mass Enthalpy	kcal/kg	-55.0456	-55.0456	-55.0694	-55.0694	-55.0854	-55.0854
Molar Entropy	cal/mol-K	-8.4747	-8.46406	-8.46348	-8.45277	-8.45204	-8.44125
Mass Entropy	cal/gm-K	-0.83275	-0.831646	-0.831599	-0.830475	-0.830419	-0.829262
Molar Density	kmol/cum	4.47717	4.45524	4.45356	4.43144	4.42976	4.40721
Mass Density	kg/cum	45.5631	45.3432	45.3255	45.1042	45.0863	44.8621
Enthalpy Flow	Gcal/hr	-16.683	-16.683	-19.8509	-19.8509	-22.7453	-22.7453
Average MW		10.1768	10.1775	10.1774	10.1782	10.178	10.1792
- Mole Flows	kmol/hr	29781.2	29779.1	35418.8	35415.8	40568.7	40563.9
H2	kmol/hr	18583.4	18580.3	22099.5	22095	25310.4	25303.2
N2	kmol/hr	5479.74	5478.68	6516.39	6514.88	7463.01	7460.64
CH4	kmol/hr	982.779	982.779	1168.89	1168.89	1338.94	1338.94
AR	kmol/hr	684.967	684.967	814.681	814.681	933.197	933.197
H3N	kmol/hr	4050.24	4052.35	4819.36	4822.38	5523.17	5527.92
WATER	kmol/hr	0	0	0	0	0	0

With his constants, there is no reaction.

On Thu, Mar 7, 2024 at 10:55 AM Sigurd Skogestad <sigurd.skogestad@ntnu.no> wrote:

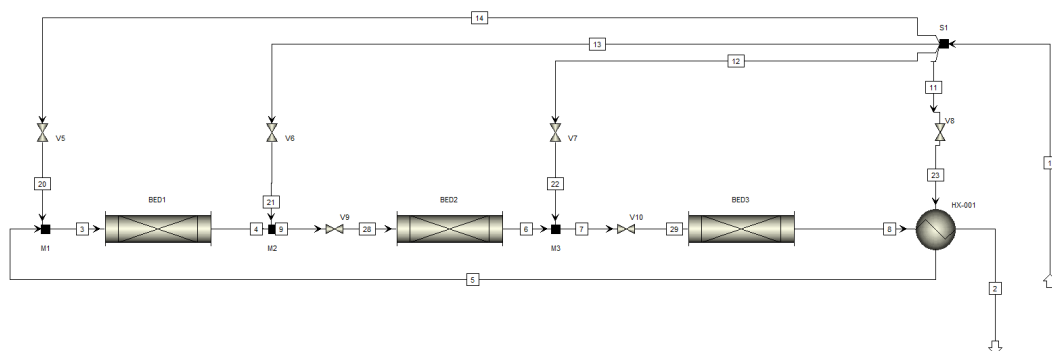
Hello

It's unclear to me what you are saying.,

From: Antonio Brandão <brandao@eq.ufcg.edu.br>
Sent: Thursday, March 7, 2024 2:37 PM
To: Sigurd Skogestad <sigurd.skogestad@ntnu.no>
Subject: Re: Letter to Editor - <https://doi.org/10.1016/j.compchemeng.2008.03.001>

Hello Sigurd.

I've done as you asked. I removed the separation section and ran simulations with the kinetic constant he obtained, keeping the feed 1 and split fractions to cold shots as before:



The conclusion is that there is no reaction whatsoever (stream 1 is the feed and 2 product):

// You get this result if you divide our old k by a factor 2950?

You are saying that their simulations are wrong?

	Units	1	2
Phase		Vapor Phase	Vapor Phase
Temperature	C	231.7	232.15
Pressure	bar	203.194	195.994
Molar Vapor Fraction		1	1
Molar Liquid Fraction		0	0
Molar Solid Fraction		0	0
Mass Vapor Fraction		1	1
Mass Liquid Fraction		0	0
Mass Solid Fraction		0	0
Molar Enthalpy	kcal/mol	-0.561707	-0.561844
Mass Enthalpy	kcal/kg	-55.1951	-55.1951
Molar Entropy	cal/mol-K	-8.50918	-8.43272
Mass Entropy	cal/gm-K	-0.836139	-0.828423
Molar Density	kmol/cum	4.54176	4.38741
Mass Density	kg/cum	46.2204	44.6605
Enthalpy Flow	Gcal/hr	-22.7906	-22.7906
Average MW		10.1768	10.1792
+ Mole Flows	kmol/hr	40573.8	40563.9
- Mole Fractions			
H2		0.624	0.623786
N2		0.184	0.183923
CH4		0.033	0.033008
AR		0.023	0.0230056
H3N		0.136	0.136277
WATER		0	0

Morud's has always been the benchmark. To try to be more convincing and avoid high conversion at the first few centimeters, my guess is that the factor f must be adjusted from the original 4.75 to fit Morud's. For that to happen, Morud's conditions must be replicated in Aspen and f adjusted accordingly, and then hope to get similar mass and energy balances, plantwide results, and dynamic behavior. This is too much work, and right now I'm very (extremely) busy.

Frankly, I think whatever comes out the same CVs will be selected in both modes. Maybe dynamics will change a bit...

Regards.

Antonio

On Thu, Mar 7, 2024 at 3:33 AM Sigurd Skogestad <sigurd.skogestad@ntnu.no> wrote:

Hello Antonio.

Yes, this is the same as you wrote last year. But it seems as strange because it seems like you should divide by ρ_{cat} and then it will get this low number. Is it possible for you to check Aspen again?

Best wishes, Sigurd.

Sent from my iPhone

6. mar. 2024 kl. 19:32 skrev Antonio Brandão
<brandao@eq.ufcg.edu.br>:

Hello again.

I'm not sure whether the pre-exponentials should be divided by ρ_{cat} , or whether the Aspen internal engine does it internally... As far as I remember, I think when I did divide by ρ_{cat} , H2 conversion was too small and the whole thing did not make any sense, as compared to a previous study.

By Morud (1998), H2 conversion in the first bed was about 10-13%. By dividing by ρ_{cat} I found a value extremely lower than that (do not remember the figure). I suspected there was something strange with Aspen's computation. I think I did not find what it was. I decided to drop the division by ρ_{cat} . Then, the conversion went up to about 20%, and I was ok with it.

Regards.

Antonio

On Wed, Mar 6, 2024 at 12:11 PM Sigurd Skogestad
<sigurd.skogestad@ntnu.no> wrote:

From: Antonio Brandão <brandao@eq.ufcg.edu.br>
Sent: Wednesday, March 6, 2024 3:09 PM
To: Sigurd Skogestad <sigurd.skogestad@ntnu.no>
Subject: Re: Letter to Editor -
<https://doi.org/10.1016/j.compchemeng.2008.03.001>

Hello Sigurd.

I could not identify the attachment. Could you please relay it to me?

Regards.

Antonio

On Wed, Mar 6, 2024 at 10:44 AM Sigurd Skogestad
<sigurd.skogestad@ntnu.no> wrote:

Hello Antonio

Can you please make a draft reply to this email

-Sigurd

From: Antony J C, Nathaniel (ELS-CHN)
<n.antonyjc@elsevier.com>
Sent: Wednesday, March 6, 2024 1:50 PM
To: Sigurd Skogestad <sigurd.skogestad@ntnu.no>; Sigurd Skogestad <sigurd.skogestad@ntnu.no>;
antonio.araujo@chemeng.ntnu.no
Cc: Ana Póvoa <apovoa@tecnico.ulisboa.pt>; Gao, Carla (ELS-BEI) <Carla.Gao@Elsevier.com>
Subject: Letter to Editor -
<https://doi.org/10.1016/j.compchemeng.2008.03.001>

Dear Authors,

This is regarding your published article “Control structure design for the ammonia synthesis process”

I would like to inform you that one of the readers has proposed to publish a ‘letter to the editor’ based on the corrections in your article.

I request you to verify the attached file and let me know your comments if any.

Regards,

Nathaniel Antony J C
Journal Manager

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