Outlook

AW: [EXT] Temperature profiles in distillation colums // Help for master's thesis

From Weber, Aaron <aaron.weber@rwth-aachen.de>
Date Mon 2024-10-28 08:04
To Lena Raenger <lena.raenger@basf.com>
Cc Sigurd Skogestad <sigurd.skogestad@ntnu.no>; mohammad.elwajeh@avt.rwth-aachen.de <mohammad.elwajeh@avt.rwth-aachen.de>; Thomas Grützner <thomas.gruetzner@uni-ulm.de>

Dear Lena,

thank you for your quick response! I will be happy to send you my thesis when it is finished at the end of February.

That answers my question! For slightly higher recoveries, I get temperature profiles that fit yours well. I also realised that the temperature profile is very sensitive at this operating point. Since i do not calculate the Vmin diagams using Underwood's equations, I will define the Vmin border by specifying the recoveries. This will hopefully allow me to construct a Vmin diagram for a non-ideally mixture.

It is good that you mention the second point. Initially I wondered why you specified the vapour flow from the bottom stage (VB), but defined the vapour flow from the top stage (VT) as a degree of freedom. When I started working with Aspen Plus, my question was answered right away, since only VB can be set as an input. I specify VB and let Aspen Plus give me the calculated VT (which differs slightly form VB) and used this to construct the Vmin diagrams. I think I got that right already.

And also thank you for sharing your simulation results with me!

Best regards

Aaron

Von: Lena Raenger <lena.raenger@basf.com>
Gesendet: Samstag, 26. Oktober 2024 12:43:27
An: Weber, Aaron
Cc: sigurd.skogestad@ntnu.no; mohammad.elwajeh@avt.rwth-aachen.de; Thomas Grützner
Betreff: RE: [EXT] Temperature profiles in distillation colums // Help for master's thesis

Dear Aaron,

Feel free to call me by my first name. Nice to hear that someone continues the work! I would be glad to receive your thesis when it is done.

Regarding your question: In the ternary feed case I did not work with recoveries directly, I used the values from the Vmin diagram as input. For the preferred split, the ideally calculated minimum was a bit off, which was visible from the temperature profile, so I adjusted it correspondingly. Looking at your profiles, it seems like my simulations had a bit higher recoveries than the ones you used (as the pinch at the top and bottom end are a bit longer).

Unfortunately, I don't have access to Aspen Plus at the moment and cannot open my simulations anymore, but I attached the backup files of some simulation I used for Figure 9 in the paper. Feel free to check them out to track the reason for the differences. So, one option is that my recoveries were higher in the ternary simulations. A second thing that you could doublecheck is if there is a difference between the vapor and the top and at the bottom of the column. In the ideal case the flow is constant, but also for a close to ideal mixture like the BTX one this is not 100% true. The Vmin diagram shows the vapor flow at the top and I usually read the one from the top end from the simulations. In Aspen Plus you can only use the vapor flow at the bottom end as input. So these two values may differ a bit.

Nevertheless, your temperature profiles already show the same characteristics in terms of pinch locations like the ones from the paper. As the length of the pinches is very sensitive to small input changes, only a small adjustment will lead to a fit. Let me know if you found the reason for the deviation and if you have further questions, please ask!

Best regards

Lena

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From: Weber, Aaron <aaron.weber@rwth-aachen.de>
Sent: Friday, October 25, 2024 11:21 AM
To: Lena Raenger <lena.raenger@basf.com>
Cc: sigurd.skogestad@ntnu.no; mohammad.elwajeh@avt.rwth-aachen.de
Subject: [EXT] Temperature profiles in distillation colums // Help for master's thesis

Dear Mrs. Ränger,

my name is Aaron Weber, and I'm currently working on my master's thesis at RWTH Aachen University, specifically at Systemverfahrenstechnik (SVT) which is part of Aachener Verfahrenstechnik (AVT). My supervisor Mohammad El Wajeh got the idea for the topic of my thesis from your paper published earlier this year. The topic of my thesis are temperature profiles in distillation columns under different scenarios such as the

consideration of pressure losses, a rather non-ideal behavior of the components and temperature profiles under dynamic conditions.

At the moment, I am working on reproducing the Vmin diagrams, based on simulation results only. To do this, I have connected Aspen Plus with MATLAB using an interface. For the simulation I am using a RadFrac model, with the same settings you did (Property method, databanks, amount of stages etc.). I have reached the point where I can determine the vapor flow from the reboiler and the distillate rate that satisfy specified recoveries. To determine the operation points at the Vmin boundary I have set a target recovery of 99.8% for the key components in each stream. The resulting Vmin diagram matches yours well. The resulting temperature profiles, however, still show deviation from those presented in the literature. In order to illustrate my results I attached two pdf files to this email, where I overlayed your results with mine. One is showing the Vmin diagram for the ternary case and the other the resulting temperatuere profiles at the "mountain peaks" (As a note, the Vmin diagram I calculated is based solely on the results of simulations. Hence the deviation in the valley of the "preferred split", that is based on ideal assumptions. However, the point b2 you found agrees well with my result).

Given this, I was hoping to ask about the framework you used for your research. Did you employ a particular software or method that might be influencing the results? Was a recovery of 99.8% for the key components the same recovery you defined as "pure" at the Vmin boundary?

You will probably be sufficiently busy designing real distillation columns with a non-infinite number of stages at BASF. Nevertheless, I would be pleased to receive an answer.

Best regards,
Aaron Weber