13.03.2024

We would like to thank the Editor for the opportunity to reply to the query raised by Dr. Aaron Drews.

Dr. Drews is indeed correct in that our pre-exponential constants are about 3000 too high. This means that we will approach equilibrium at the exit of the reactor. Fortunately, the error seems to have little impact on the results in our paper because equilibrium is also reached with the much lower corrected value of Drews.. This is shown with a simulation for the two cases (see figure) with feed flow rate at 252,000 kg/h, feed temperature at 250 oC, feed pressure at 200 bar, and mass fraction of ammonia at 0.08. This corresponds to the upper steady state from Morud and Skogestad, 19951. There is a large difference in bed 1, but the exit conditions from bed 3 are close to equilibrium and therefore almost the same.



Antonio Brandao Araujo and Sigurd Skogestad

16 Nov. 2024:

I'm a bit confused here. Didn't we already submit a response to a similar Letter to the Editor in March 2024? Wasn't it published?

Our response was that then that there was an error in the kinetics but that it doesn't effect the results in the paper because we are anyway close to equilibrium at the outlet.

I continued to work on ammonia reactors and I know that equilibrium is what one normally achieves in industrial reactors, except when close to changing catalyst (which may be after 5 years). So in conclusion, the results from our paper are nit affected by the error.

I Dr. Drews last letter he says with the "correct" data one achieves conversion of about 0.3% in the first bed. I can say that this for sure is completely unrealistic in industrial reactor, so maybe the problem stems from errors within Aspen. Actually, this may be way we "omitted" the rho in 2008 because with the "correct" kinetics the Aspen results made no sense.

Sigurd Skogestad