

Correction to “Analysis of Membrane and Adsorbent Processes for Warm Syngas Cleanup in Integrated Gasification Combined-Cycle Power with CO₂ Capture and Sequestration”

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Supporting Information

The pressure swing adsorption models used in ref 1 were incorrect, because they involved the use of a co-current rinse step with pure steam above its dew pressure, yielding unphysical results. These models have been corrected to include an extra depressurization step to first lower the total pressure of the column below the dew point of the steam. The new cycle consists of six steps: pressurization, adsorption, co-current depressurization, co-current rinse, countercurrent depressurization, and countercurrent desorption. Furthermore, we have replaced our original linear driving force (LDF) rate expression [$rate = k_{LDF}(q^* - q)$] with one based on the difference between the bulk gas concentration and concentration in equilibrium with the sorbent bed [$rate = k_{LDF}(C - C^*)$], following the method of Seader and Henley.² The former rate expression is widely used,^{3,4} but we feel the method of Seader and Henley more accurately reflects the limiting behavior of the adsorption rate.

The corrected model slightly changes Figures 19–27, but the optimal $|\Delta H_{ads}|$ remains unchanged at 65 kJ/mol. With the corrected model, the maximum efficiency achieved in adiabatic operation is 31.9% (down from the originally reported 32.7%), and the maximum efficiency achieved in isothermal operation was unchanged at 33.2%. We have included these corrected models in the Supporting Information for this correction. The results of the membrane calculations were unaffected.

■ ASSOCIATED CONTENT

Supporting Information

The authors have provided Aspen Plus files and detailed documentation for the CO₂ pressure swing adsorption models (adiabatic and isothermal models for steam regeneration and H₂ regeneration), as well as all necessary Excel and MATLAB files. This material is available free of charge via the Internet at <http://pubs.acs.org/>.

■ REFERENCES

- (1) Couling, D. J.; Prakash, K.; Green, W. H. *Ind. Eng. Chem. Res.* **2011**, 50, 11313–11336.
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- (3) Yang, R. *Gas Separation by Adsorption Processes*; Imperial College Press: London, 1997.
- (4) Simo, M.; Brown, C. J.; Hlavacek, V. *Comput. Chem. Eng.* **2008**, 32, 1635–1649.

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