



# Process and Material Design for Micro-Encapsulated Ionic Liquids in Post-Combustion CO<sub>2</sub> Capture

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# **Outline**

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- Results
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  - Sensitivity of Microcapsule diameter
- Concluding remarks

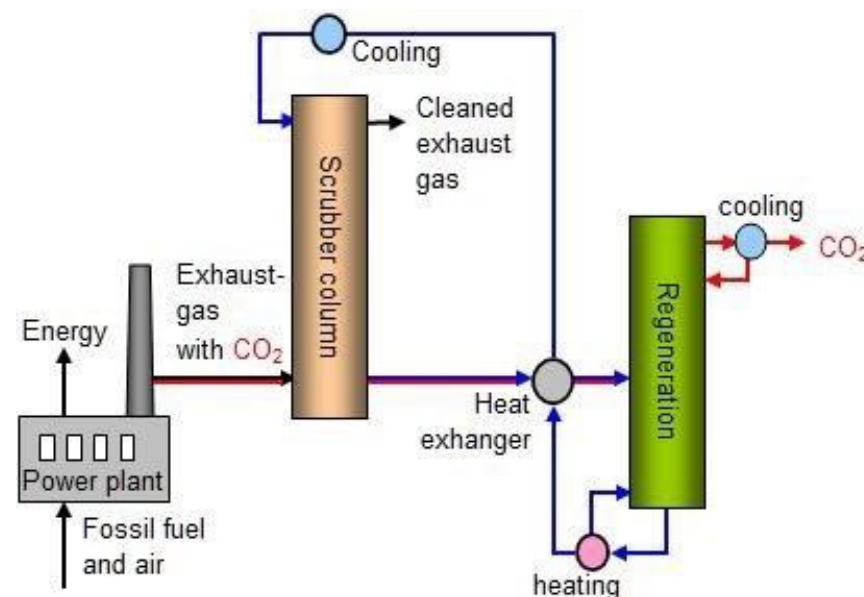
Background

# ***Ionic Liquids for CO<sub>2</sub> capture (post-combustion)***

ILs are nonvolatile salts with low melting points, wide liquid phase operating ranges, and endless tunability.



- Potential advantages
  - Require no added water to serve as a diluent
  - Good thermal and oxidative stability
  - No evaporation into cleaned gas stream
- Potential disadvantages (early-generation ILs)
  - Viscosity increase after absorbing CO<sub>2</sub>
  - Low CO<sub>2</sub> capacity (physical)
- Aprotic Heterocyclic Anion (AHA) ILs offer solutions to these issues (Gurkan *et al.* 2010)

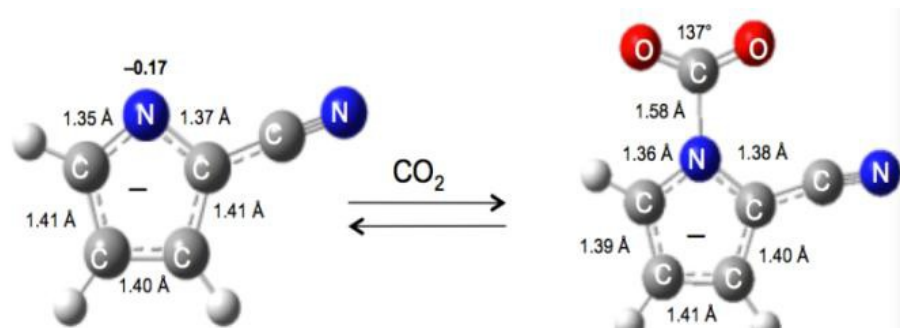


<http://www.bellona.org/factsheets/1191913555.13>

# AHA ILs -- Chemically complexing IL design for post-combustion carbon capture

## **1. Double the capacity compared to MEA**

Demonstrated experimentally that a 1:1 reaction stoichiometry is achieved<sup>1</sup>

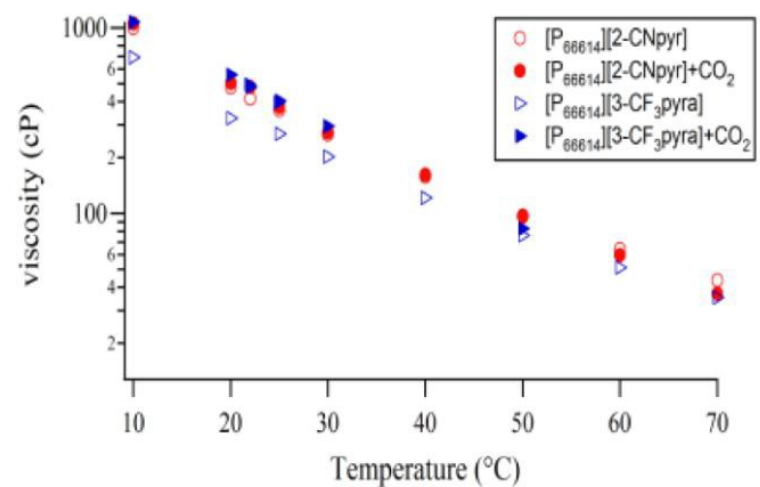


## **2. Eliminate viscosity increases**

Aprotic heterocyclic anion (AHA) can hinder the formation of the hydrogen bonding which is the main cause of IL's viscosity increases<sup>1</sup>

## **3. Optimize reaction enthalpy**

Using equilibrium-based process optimization, we identified the optimal reaction enthalpy of CO<sub>2</sub> absorption is around **- 50 KJ/mol<sup>2</sup>**



1. Gurkan, B., et al. *The Journal of Physical Chemistry Letters* 1 (2010): 3494-3499.
2. Hong, B., et al., *Industrial & Engineering Chemistry Research* 55 (2016): 8432-8449.

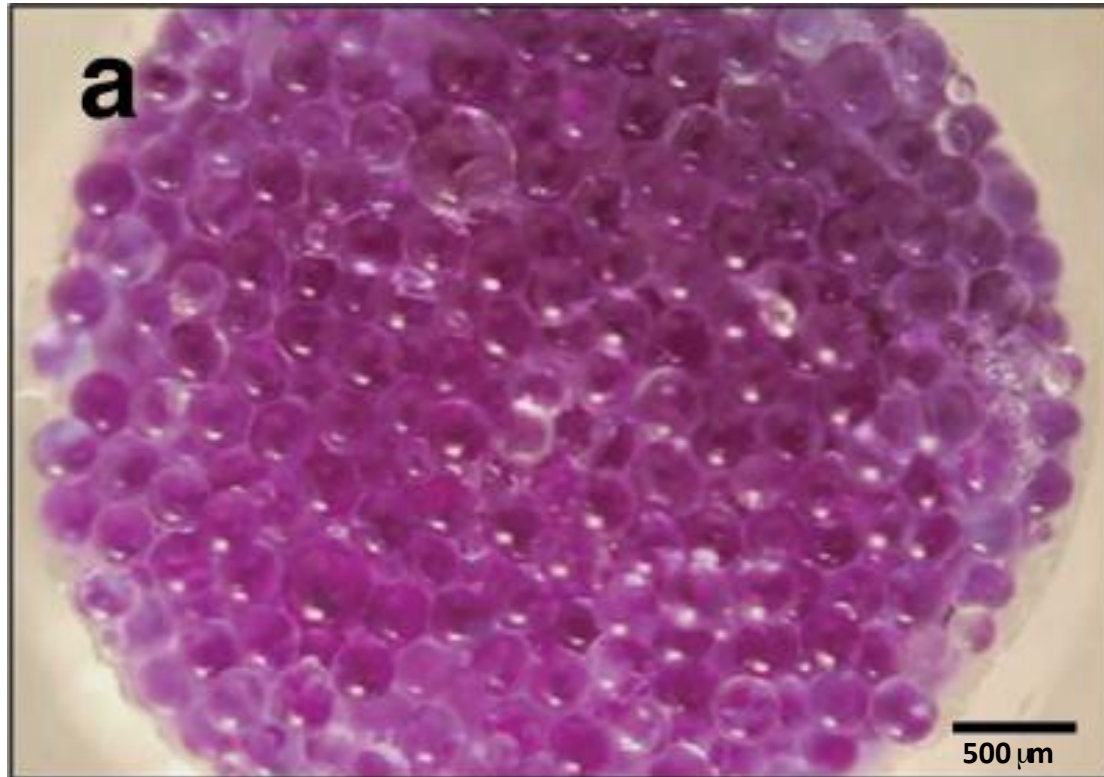
## **AHAs in a packed column absorber**

The typical viscosity of AHAs at 40 °C is 100 cP.  
This results in relatively:

- Low CO<sub>2</sub> diffusion coefficient
- Low wetted surface area
- High pressure drop

# **Microencapsulation technology**

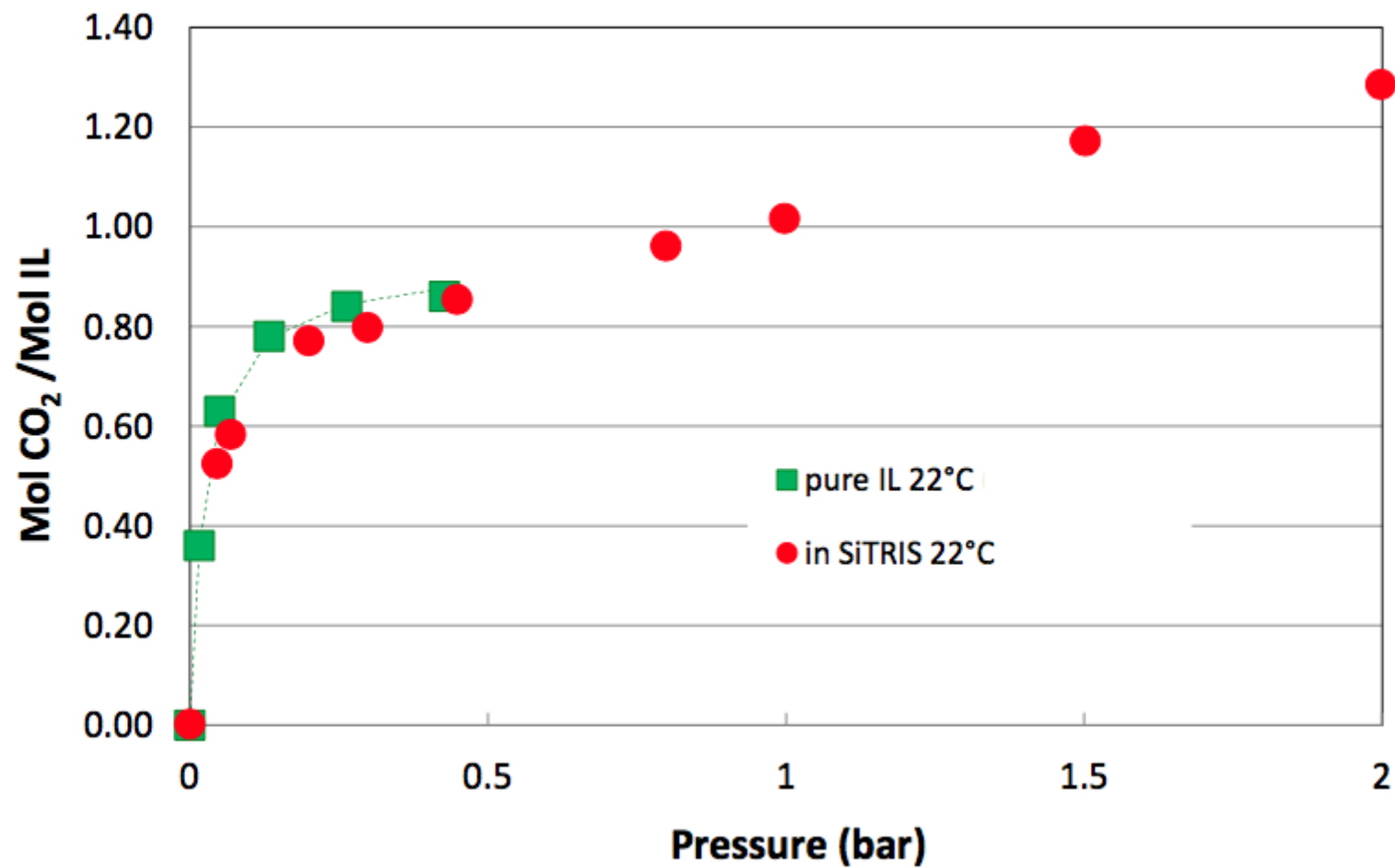
- Improve reactor productivity by increasing mass transfer area.
- Improve the reactor temperature control by fluidization.



Vericella J J, Baker S E, Stolaroff J K, et al. Nature Communications, 2015, 6:6124.

## **Encapsulated IL maintains capacity**

**Solubility of CO<sub>2</sub> in NDIL0230 in SiTRIS at 22°C**

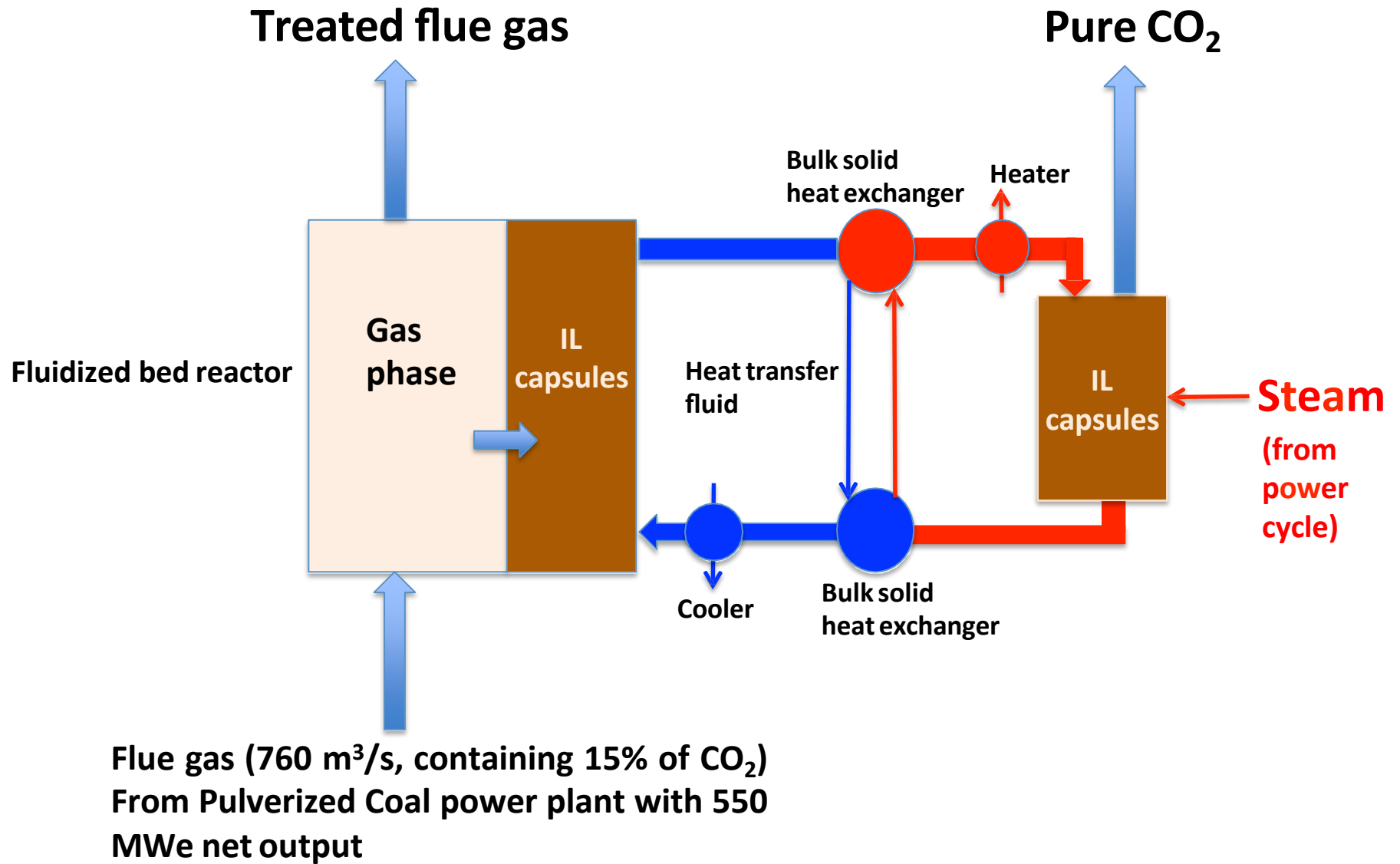


(Measured by Tangqiumei Song)



# Process design

# Process schematics



# **Process conditions (not optimized) used in analysis**

## **Process operating conditions:**

- $T_a = 308.15 \text{ K}$
- $P_a = 1 \text{ bar}$
- $T_s = 473.15 \text{ K}$
- $P_s = 1 \text{ bar}$

## **Fluidization conditions (riser type):**

- Average solid fraction = 0.1
- Exit solid fraction = 0.01
- Solid circulation rate =  $7.5 \text{ m}^3/\text{s}$

## **Flue gas conditions: (Case 10 in NETL report 2010)<sup>1</sup>**

- Flue gas flow rate = 99950 kmol/hr (after water knockout)
- $\text{CO}_2$  mole fraction : 0.15 (after water knockout)

1.Black, James. "Cost and performance baseline for fossil energy plants, Volume 1: Bituminous coal and natural gas to electricity." *National Energy Technology Laboratory: Washington, DC, USA* (2010).

## **IL properties used in analysis**

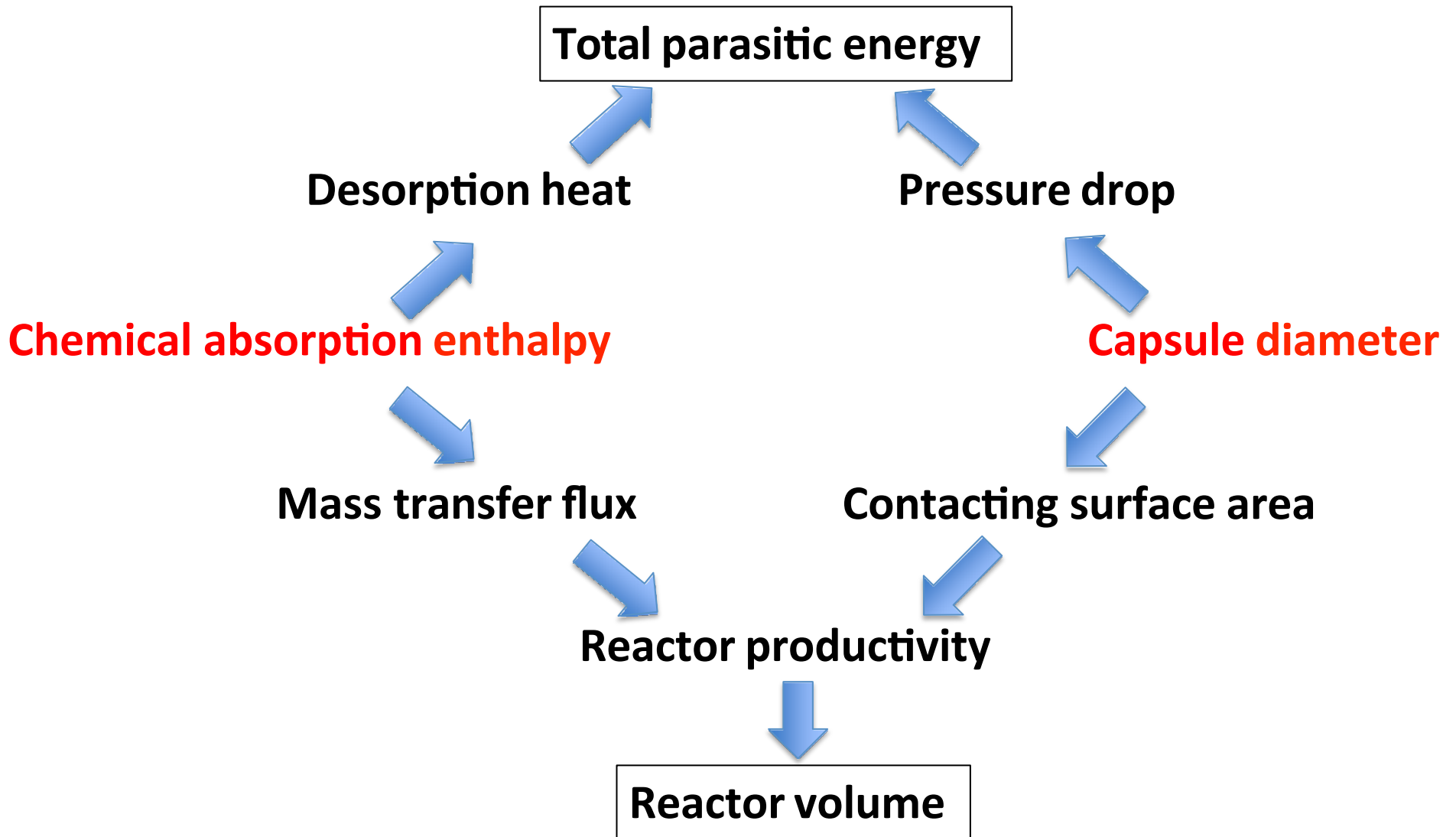
[P<sub>66614</sub>][2-CNpyr]:

- Chemical absorption entropy<sup>1</sup> =  $-130 \text{ J}/(\text{mol K})$
- IL viscosity = 100 cP
- Second order reaction rate<sup>2</sup> =  $10 \text{ m}^3/(\text{mol s})$
- IL density<sup>1</sup> =  $0.892 \text{ (g/cm}^3\text{)}$
- IL molecular weight<sup>1</sup> =  $575 \text{ (g/mol)}$

1. Seo S. et al. The Journal of Physical Chemistry B, 2014, 118: 5740-5751.

2. Gurkan B. et al. Physical Chemistry Chemical Physics, 2013, 15: 7796-7811.

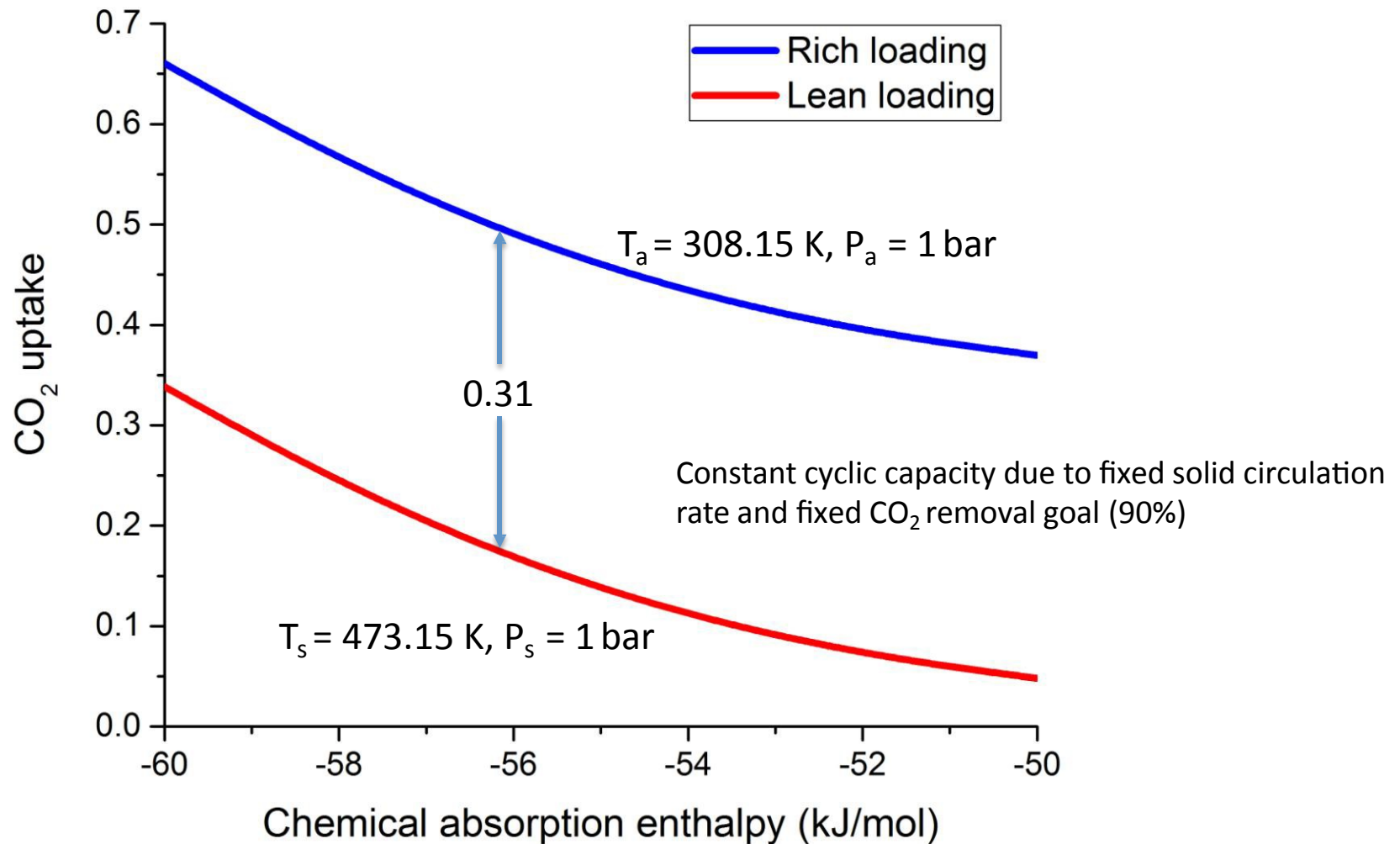
# *Process performance improvement with better engineered properties*



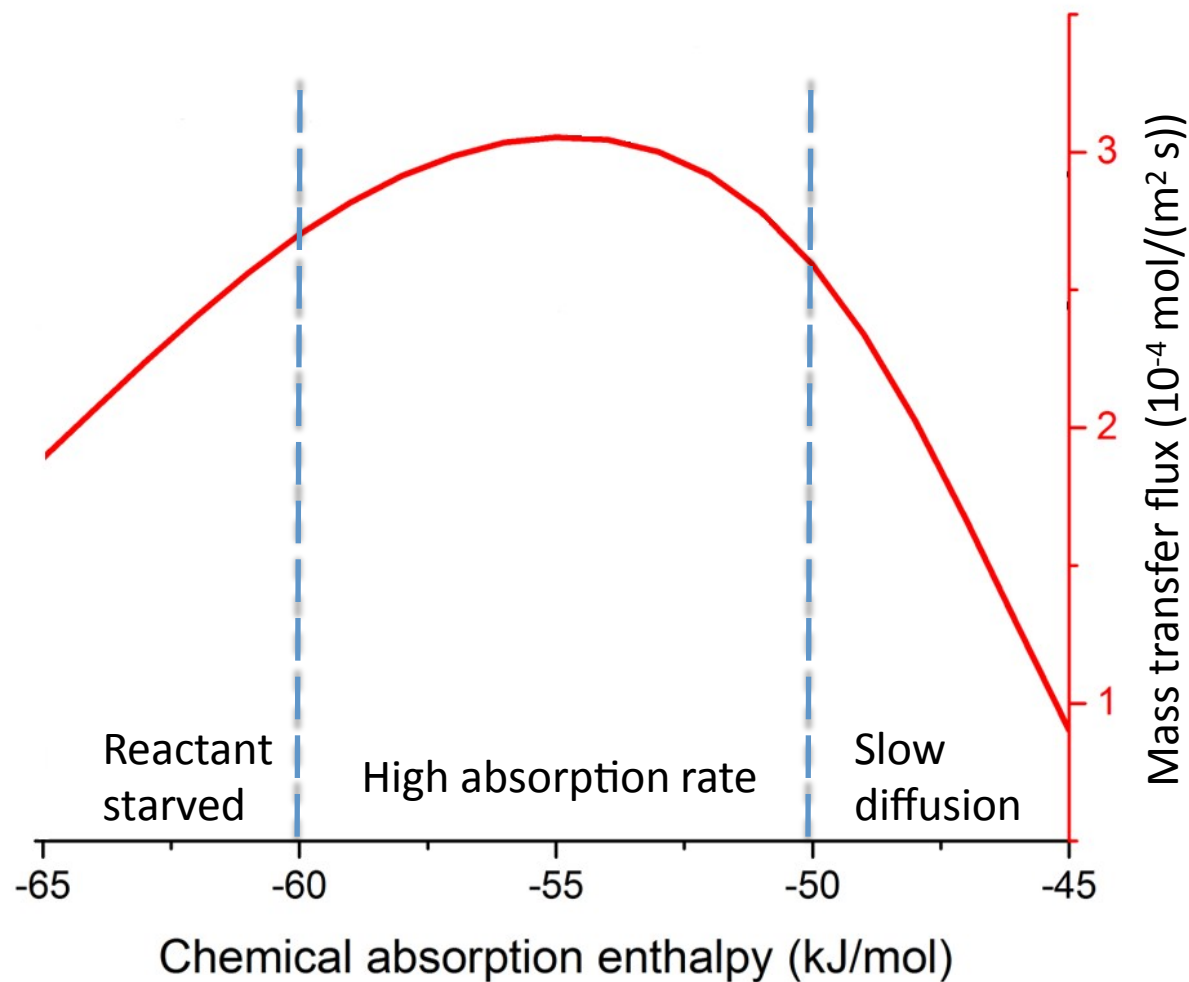
# Results

## (Chemical absorption enthalpy)

## Effect of absorption enthalpy on CO<sub>2</sub> uptake

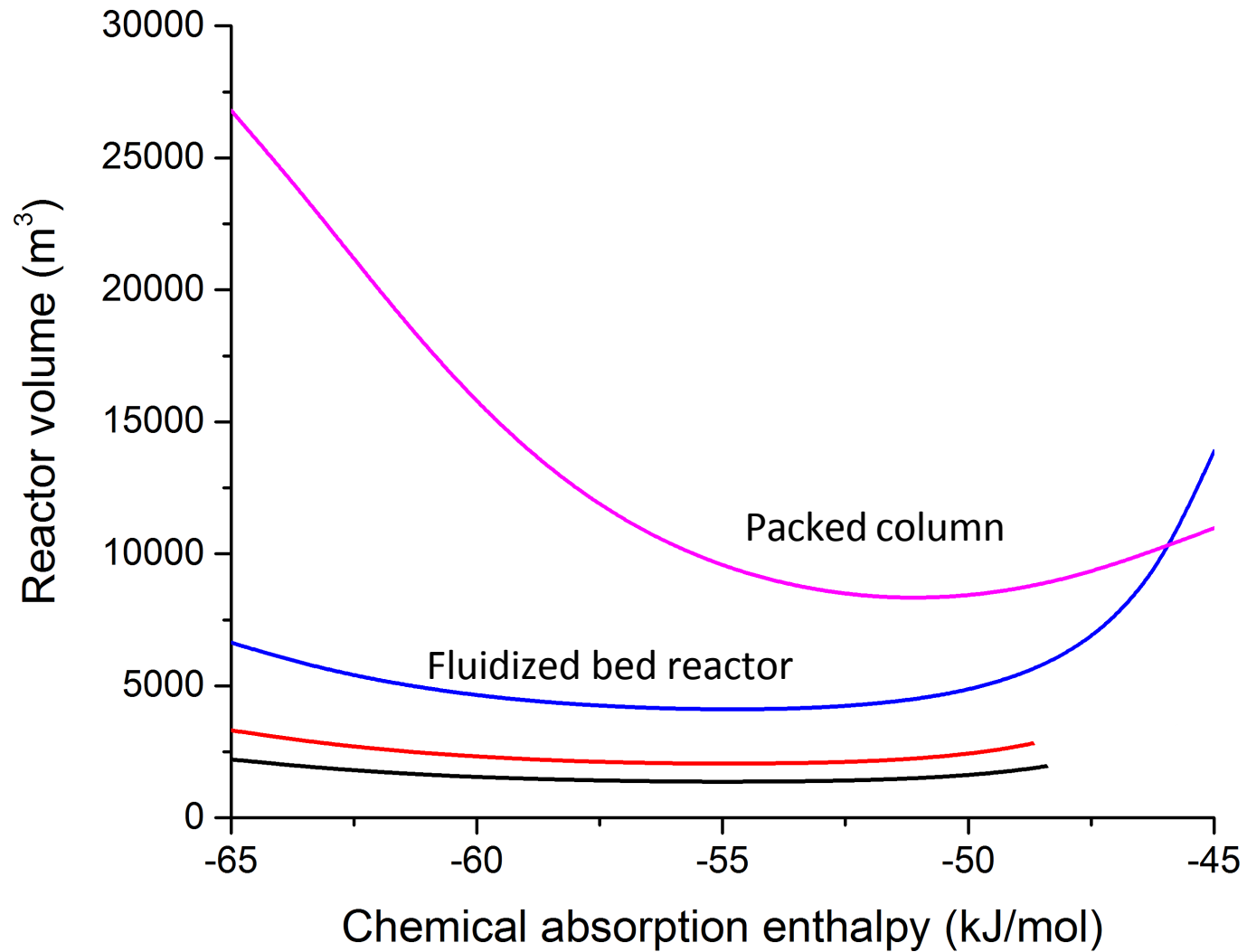


## ***Effect of absorption enthalpy on mass transfer flux***





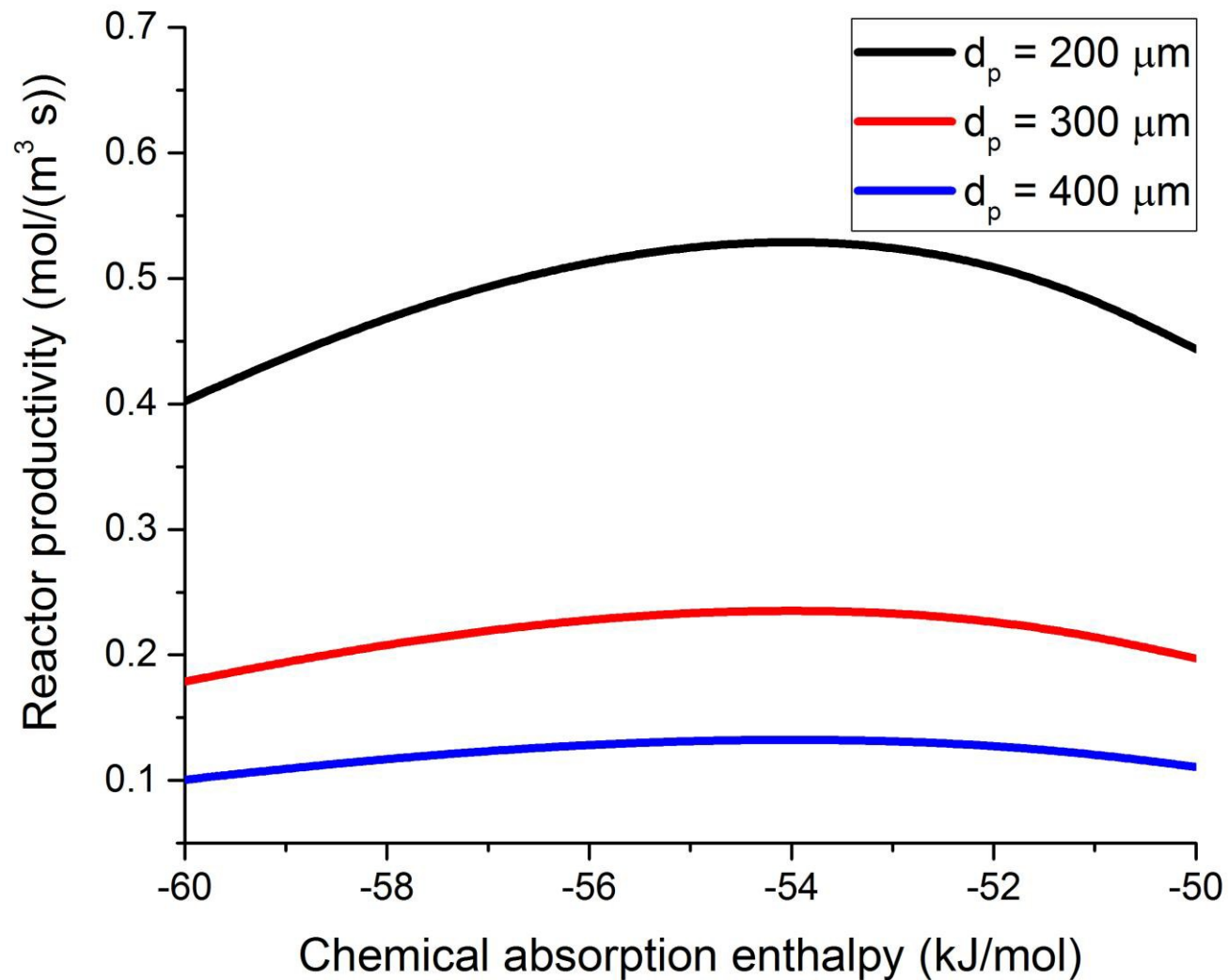
## **Packed column vs. FB reactor volume**



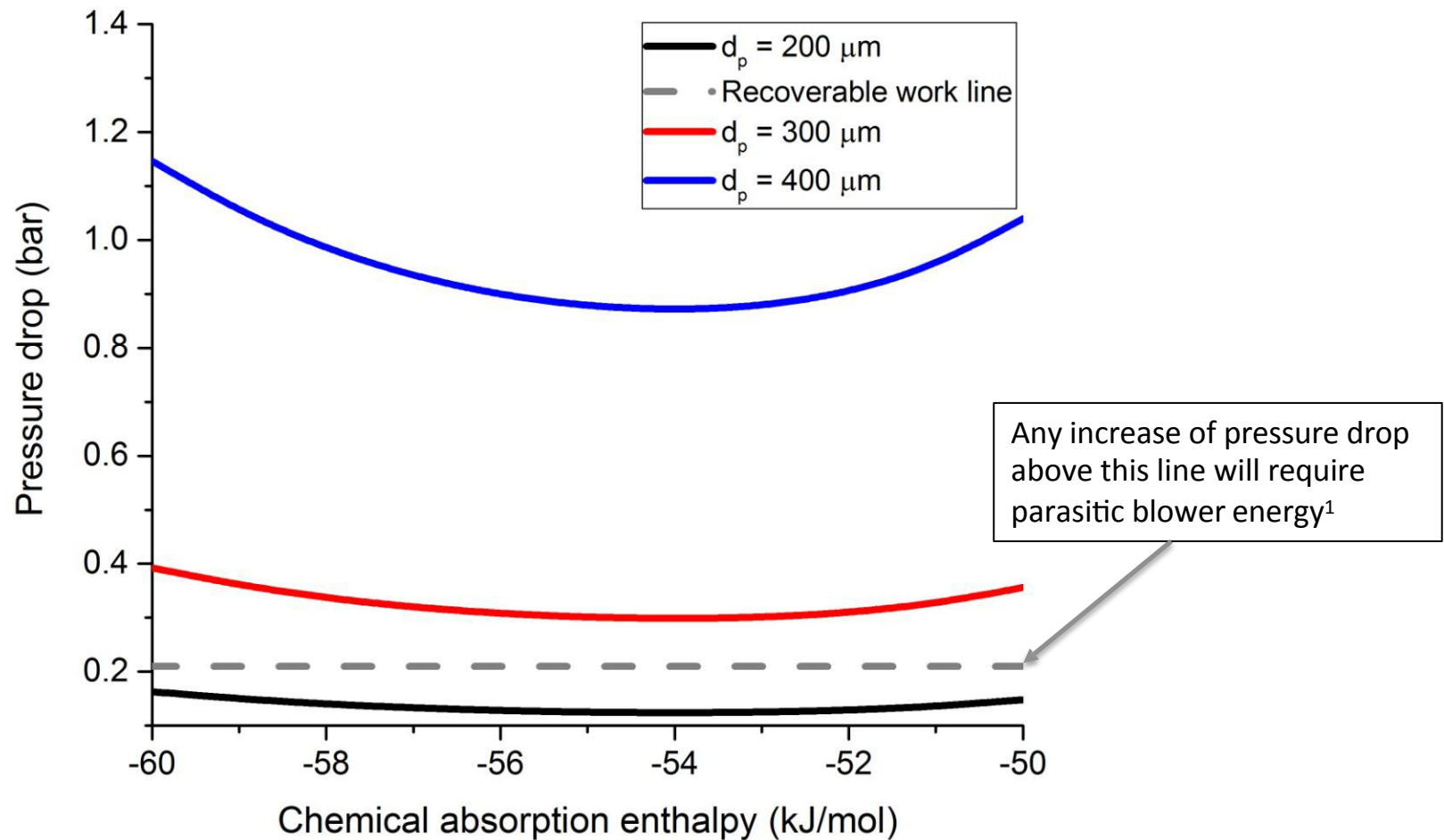
# Results

## (Capsule diameter)

## **Effect of capsule diameter on reactor productivity**

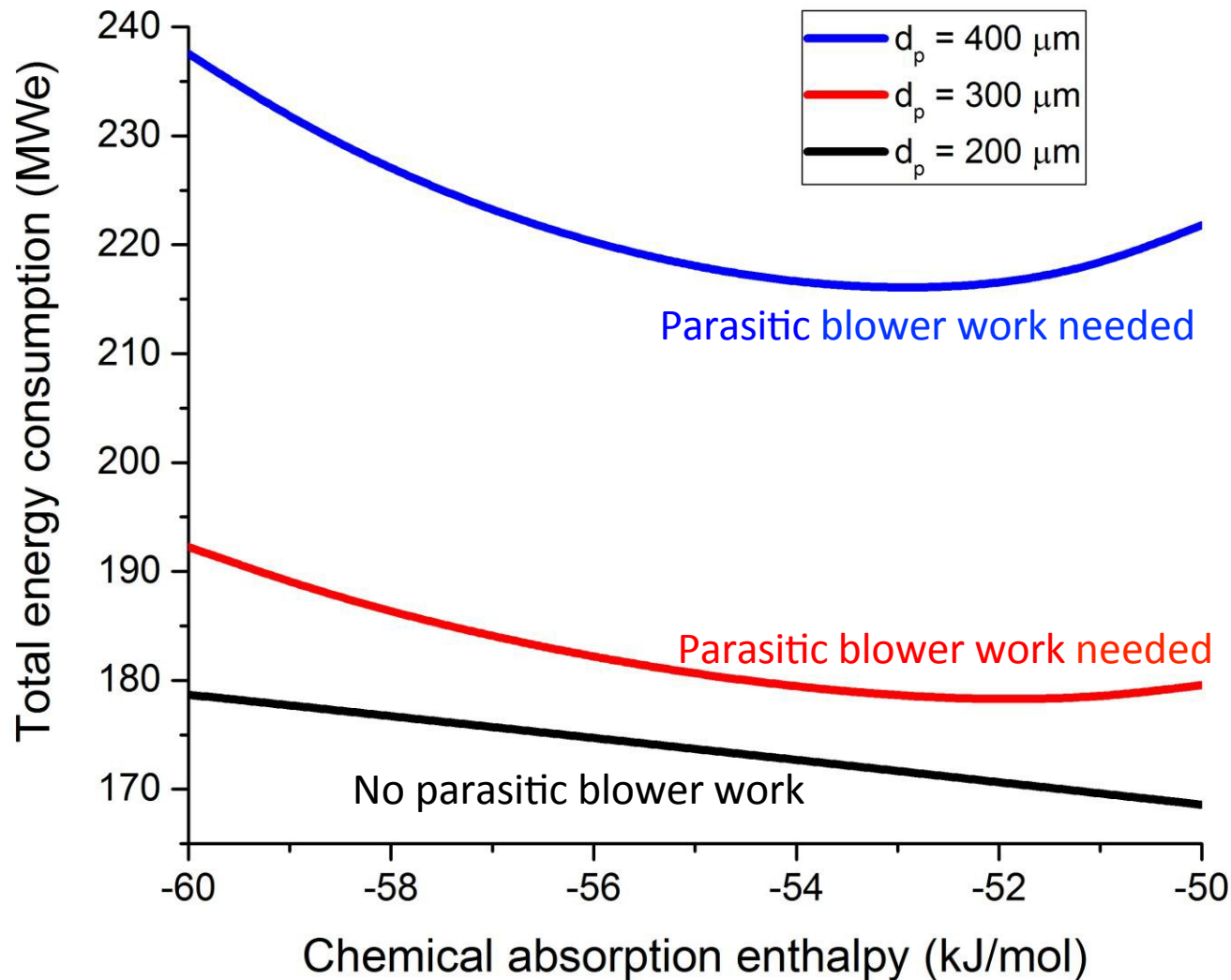


## Effect of capsule diameter on pressure drop



1. Yang, Wen-Ching, and James Hoffman. *Industrial & Engineering Chemistry Research* 48 (2008): 341-351.

## **Effect of capsule diameter on energy consumption**



Note : the numbers of energy consumption shown above are not yet optimized.

## **Concluding remarks**

- Too strong or too weak an absorption enthalpy will reduce the mass transfer flux: The optimum absorption enthalpy is around  $-55 \text{ kJ/mol}$
- A capsule diameter of 200 microns can double the productivity and halve the reactor volume compared with IL-based packed column
- A capsule diameter of 200 microns will reduce the blower work to a level that can be fully recovered from the plant-wide energy system, and thus, offset the high viscosity problem of AHAs

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