Viscosity Effects in Amine Scrubbing with 8 m 2-Methylpiperazine

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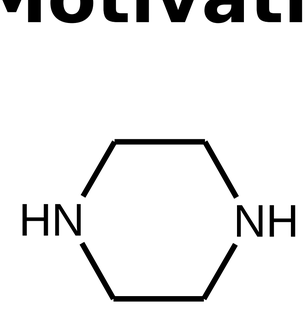
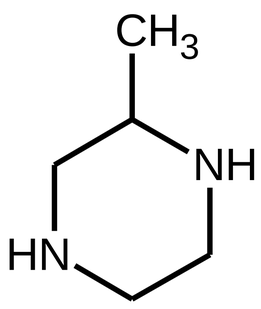
CCSI™ Carbon Capture Simulation Initiative

TXCMP

Motivation



piperazine (PZ)



2-methylpiperazine (2MPZ)

- PZ offers double the rate of MEA and 60% greater capacity
- Due to solid solubility problems of PZ, 2MPZ is proposed
- 2MPZ is fully soluble across all loading ranges

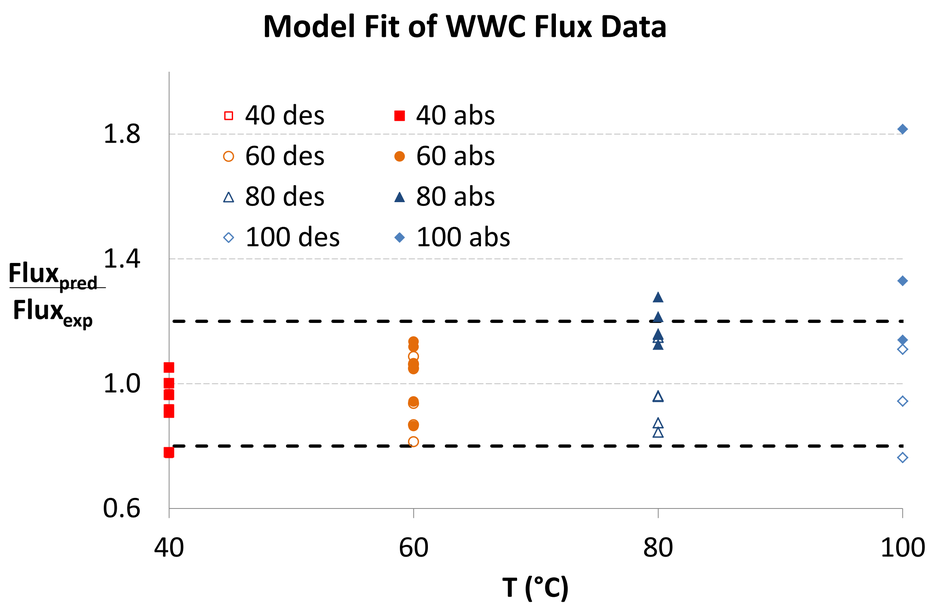
Summary

Property/Amine (m)	7 MEA	8 PZ	8 2MPZ	4 2MPZ/4 PZ
ΔC $\left(\frac{mol\ CO_2}{kg\ solvent}\right)$	0.47	0.79	0.93	0.84
ΔC_μ	0.60	0.77	0.70	0.63
μ_{rich} (cP)	3.8	11.37	31.26	30.67
Loading range $(mol/mol\ alk)$	0.45–0.55	0.31–0.39	0.27–0.37	0.30–0.39
$-\Delta H_{abs}\ (kJ/mol)^\dagger$	82	70	72	70
T_{max} (°C)	122	163	151	155
$k'_{g,avg}(10^7 mol/s-Pa-m^2)^\ddagger$	4.3	8.5	5.9	7.1

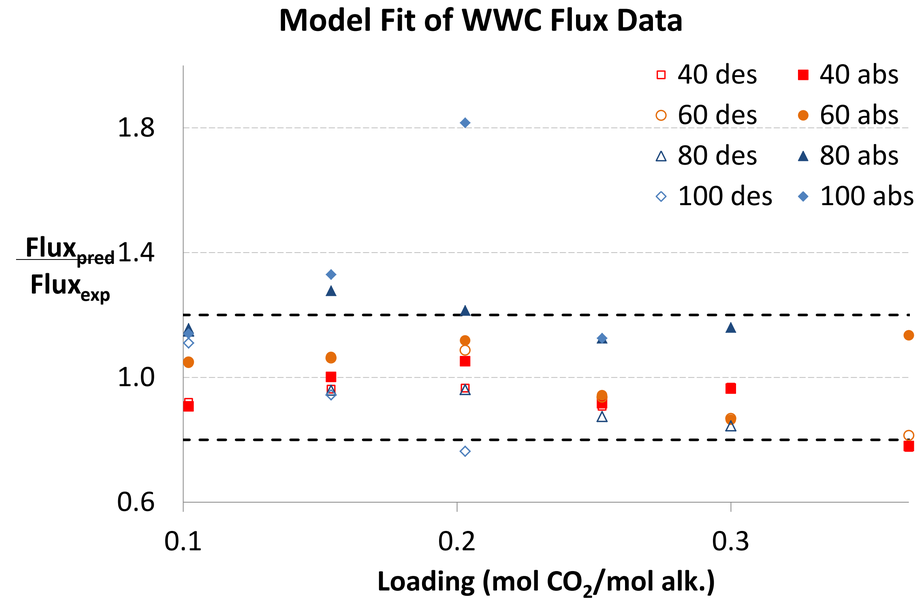
†at $P^*_{CO_2}$=1.5 kPa; ‡at 40°C

- 40% greater $k'_{g,avg}$ than MEA
- twice the capacity of MEA
- fully soluble at all loading ranges

- equal heat of absorption to MEA
- useful capacity reduced by high viscosity
- 30% slower $k'_{g,avg}$ than PZ



small linear bias fit by $\left(\frac{Flux_{pred}}{Flux_{exp}} = 0.0051T + 0.69\ ,\ R^2 = 0.28\right)$



$^{33}/_{40}$ points fit within 20%, which is accuracy of WWC

Parameter	Value
D_o	4.4E-11 m²/s
α	-1.5
β	-11.5

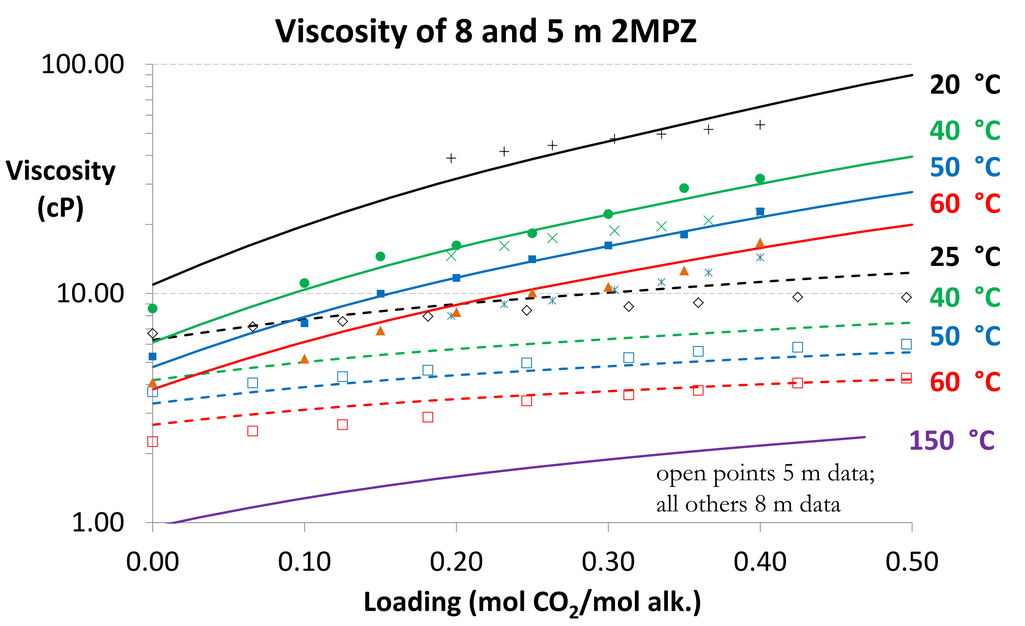
$$D_{Am} = D_0\left(\frac{T}{T_{ref}}\right)^{\beta}\left(\frac{\mu}{0.0465\text{Pa}-\text{s}}\right)^{\alpha}$$

$$k = k_0\exp\left[\left(\frac{-E_A}{R}\right)\left(\frac{1}{T}-\frac{1}{T_{ref}}\right)\right]$$

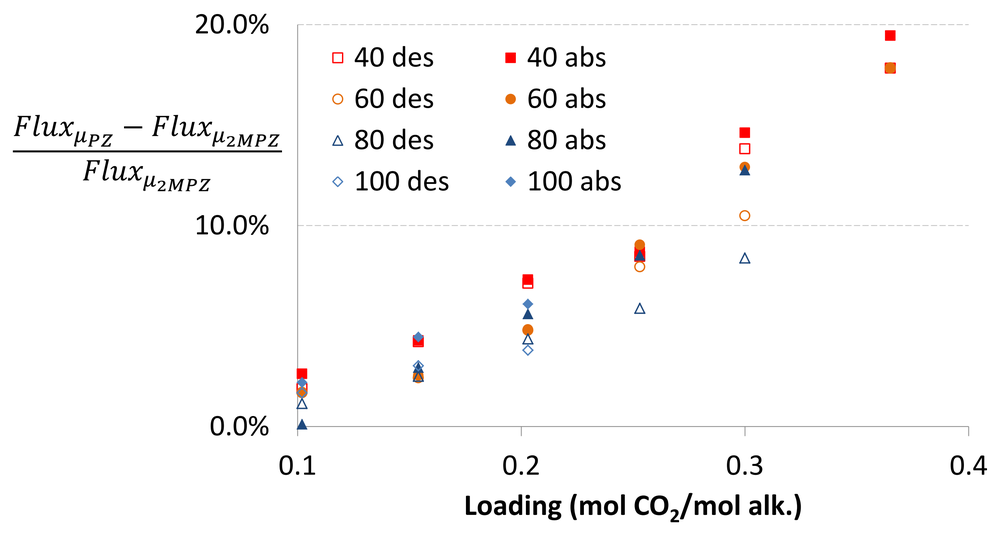
Reaction	k_o (kmol/s-m³)	E_A (10^4 kJ/kmol)
2MPZCOO + H_2O + CO_2 → H2MPZCOO + HCO_3^-	2.62×10^6	9.80
2 2MPZ + CO_2 → $2MPZH^+$ + $2MPZCOO^-$	1.45×10^{10}	2.19
2 $2MPZCOO^-$ + CO_2 → $^+H2MPZCOO^-$ + $2MPZ(COO)_2^{2-}$	1.28×10^{10}	2.19
H2MPZCOO + HCO_3^- → 2MPZCOO + H_2O + CO_2	3.67×10^5	17.4
$2MPZH^+$ + $2MPZCOO^-$ →2 2MPZ + CO_2	3.96×10^4	9.78
$^+H2MPZCOO^-$ + $2MPZ(COO)_2^{2-}$ → 2 $2MPZCOO^-$ + CO_2	2.71×10^8	12.9

Parameter	A	B	C	D	E	F	H
Value	-1.52×10^3	2.25×10^3	2.05	5.37	14.0	-5.81×10^{-3}	-1.52

$$\mu_{pure} = \mu_{H_2O}\exp\left\{\frac{\Omega[(A\Omega+B)T+C\Omega+D][(E\Omega+FT+H)\alpha+1]}{T^2}\right\}$$



best fit in the operational loading range



2MPZ rate due to steric hindrance more than μ

$P^*_{CO_2}$=5 kPa → α_{rich}; $P^*_{CO_2}$=0.5 kPa → α_{lean}

$$\Delta C = \frac{(\alpha_{rich}-\alpha_{lean})\cdot mol\ alk}{kg(amine+H_2O)} \qquad \Delta C_\mu = \Delta C \times \left(\frac{\mu}{10\ cP}\right)^{-0.25}$$