

The impact of critical model parameter correlations on the rate based model for CO₂ absorption into MEA

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Introduction & Motivation

- State of art of technology: Pilot & Industrial scale demonstration
- For detailed understanding of the process : many experimental and theoretical studies
- Scale up: from pilot to industrial scale, need accurate models to predict the system behaviour
- Several sensitivity studies had been performed
 - Most of the studies are performed using pilot scale data
- **Models: combinations of different correlations of parameters**
 - **Parameters taken from different kinds of studies**
 - Different assumptions in estimation of parameters

Introduction & motivation

[From the literature, numerical and sensitivity studies](#)

- Henry's constant, packing mass transfer coefficients and active area, Kinetic constants have high sensitivity
- With same set of correlations and by changing the kinetic constants, model predictions for CO₂ removal efficiency goes from under-prediction to over-prediction.
- Different combinations of parameter correlations gives different predictions for the same case

Study outline

- Penetration theory model is used for the study
- WWC experimental data, CO₂ absorption into 5 M MEA solution

Case studies

- Case 1: Effect of changing only Henry's law constant correlation
- Case 2: Effect of using different diffusivity of CO₂ in MEA correlations
- Case 3: Effect of using different viscosity correlations
- Case 4: Effect of different kinetic constants correlations
- Case 5: complete set of correlations

Cases

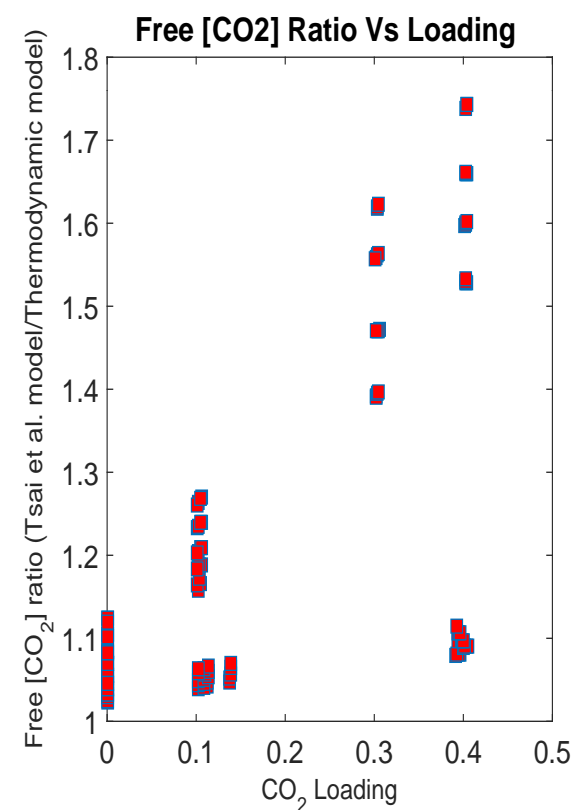
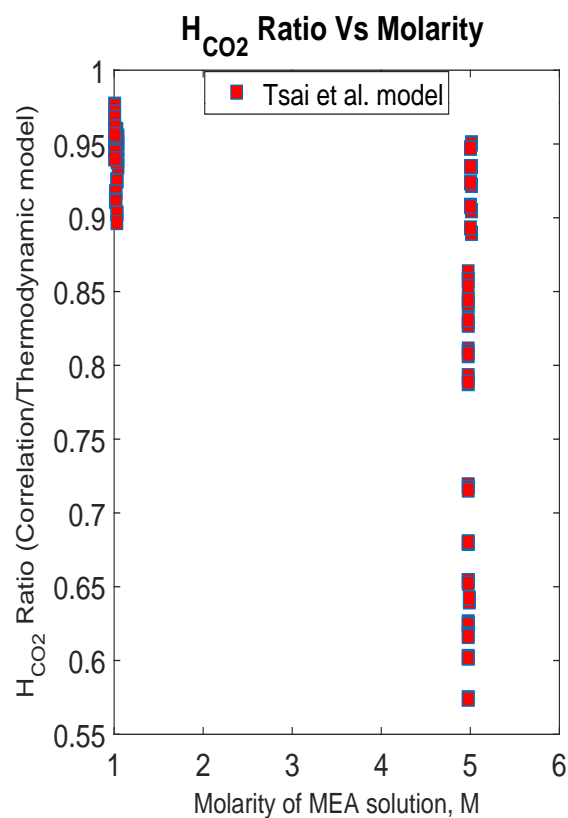
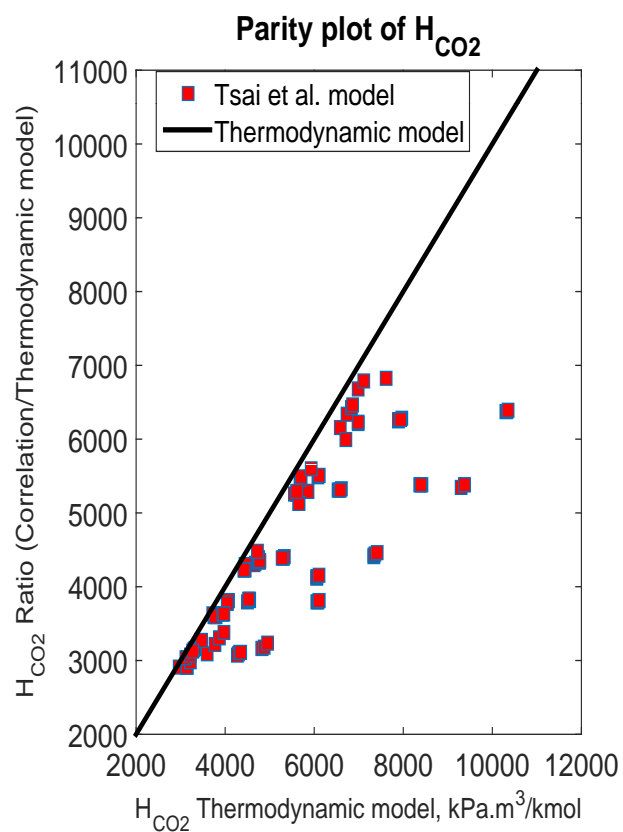
Base case	
Property	Source
Thermodynamic model	Inhouse e-NRTL model
Kinetic model	Inhouse
$D_{\text{CO}_2\text{-MEA}}$	Ko et al. (2000) based on N_2O analogy
$D_{\text{MEA-MEA}}$	Snijder et al. (1993)
Viscosity	Hartono et al. (2014)

Case 1: changing Henry's law constant correlation

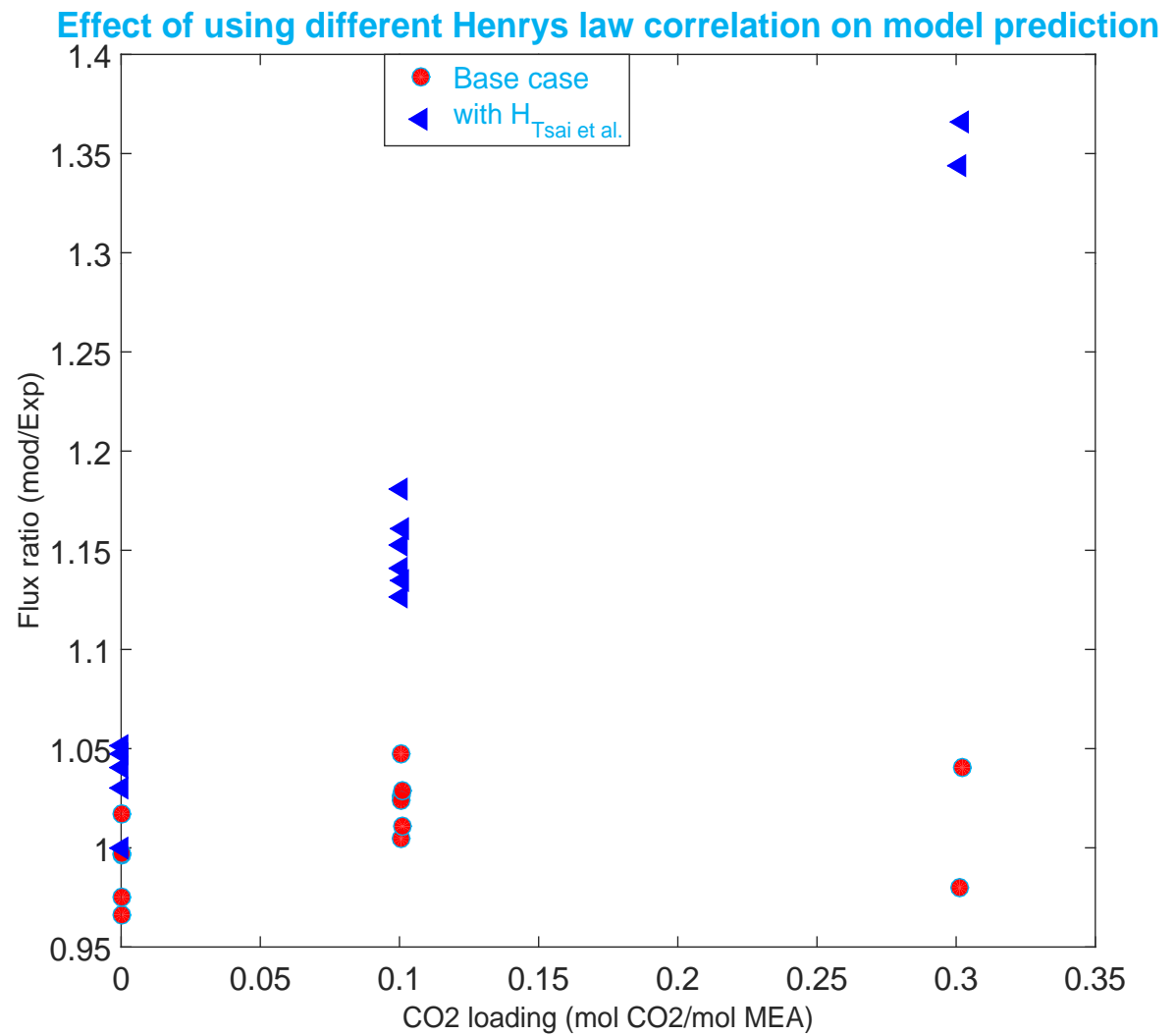
Case 1	
Property	Source
Thermodynamic model	Inhouse e-NRTL model
Kinetic model	Inhouse
$D_{CO_2_MEA}$	Ko et al. (2000)
D_{MEA_MEA}	Snijder et al. (1993)
Viscosity	Hartono et al. (2014)

Henry's constant correlation changed to **Tsai et al. (2000)**

How different are these Henry's law constant correlations??



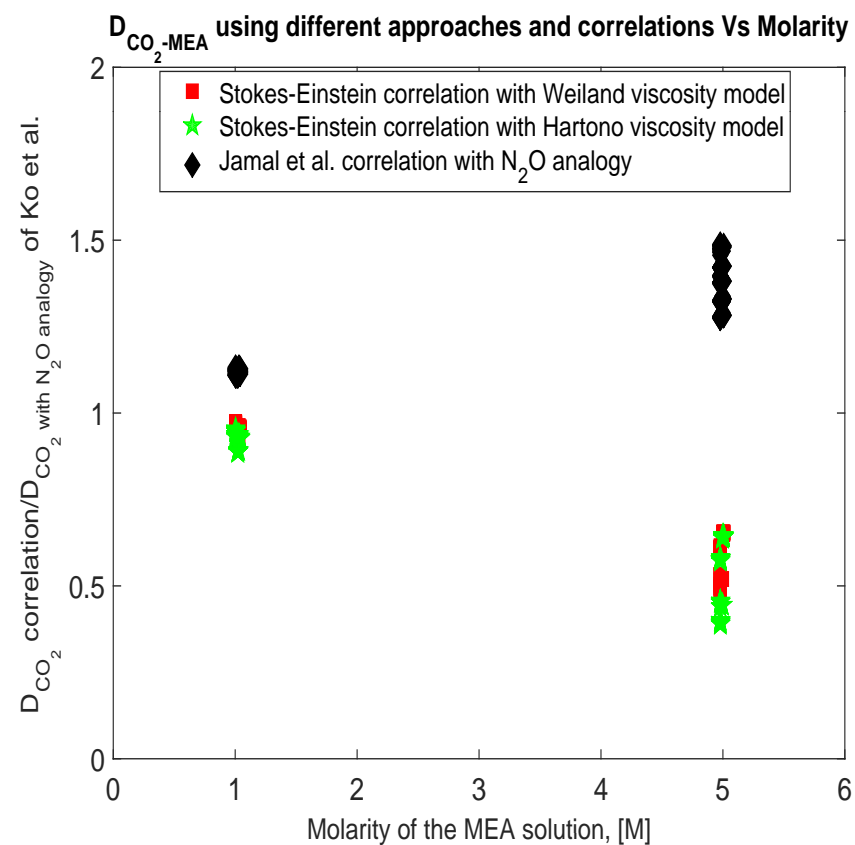
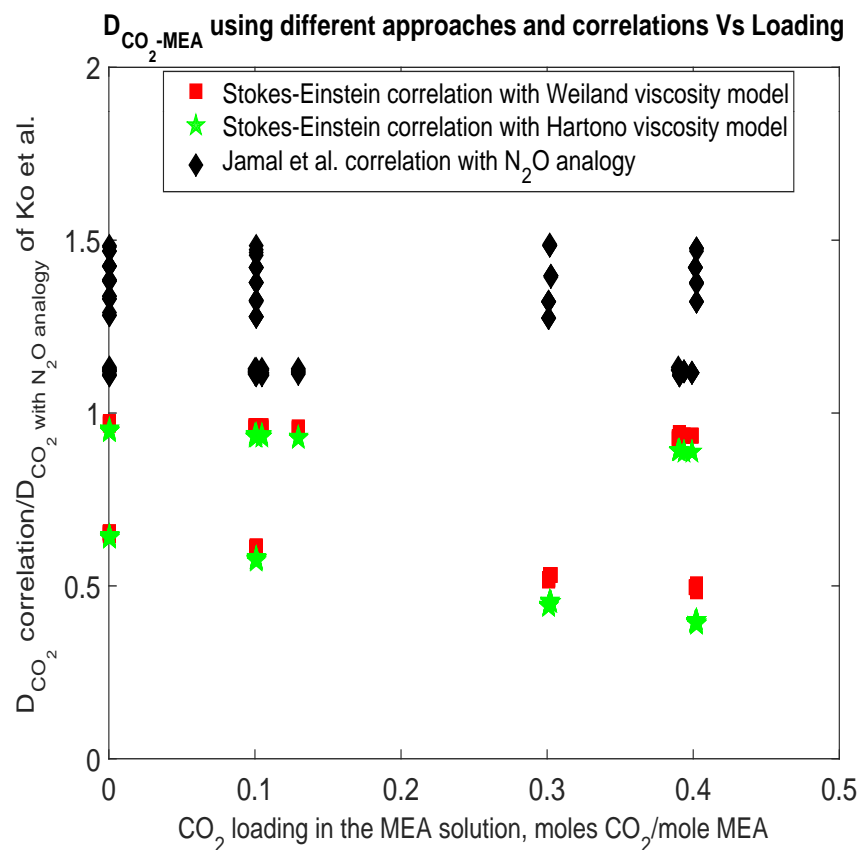
Results : Case 1



Case 2: Effect of using different diffusivity correlations for CO₂ in MEA

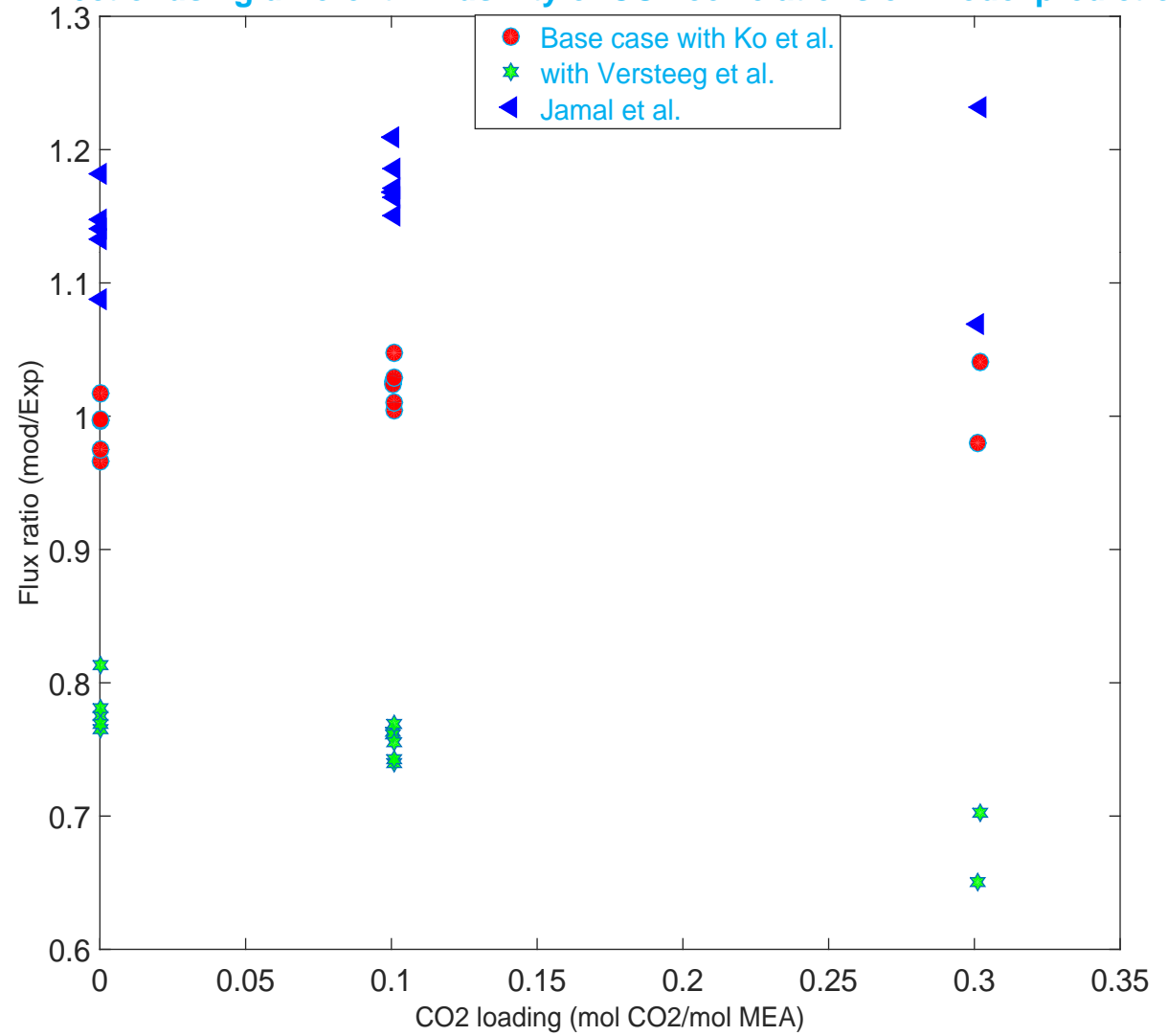
Case 2	
Property	Source
Thermodynamic model	Inhouse e-NRTL model
Diffusivity correlation changed to Versteeg et al. (1996) (based on modified Stokes-Einstein correlation) and Jamal et al. (2002) (N₂O analogy) $D_{CO_2_MEA}$	Inhouse Jamal et al. (2002) & Versteeg et al. (1996)
D_{MEA_MEA}	Snijder et al. (1993)
Viscosity	Hartono et al. (2014)

How different are these diffusivity correlations??



Results : Case 2

Effect of using different Diffusivity of CO2 correlations on model prediction

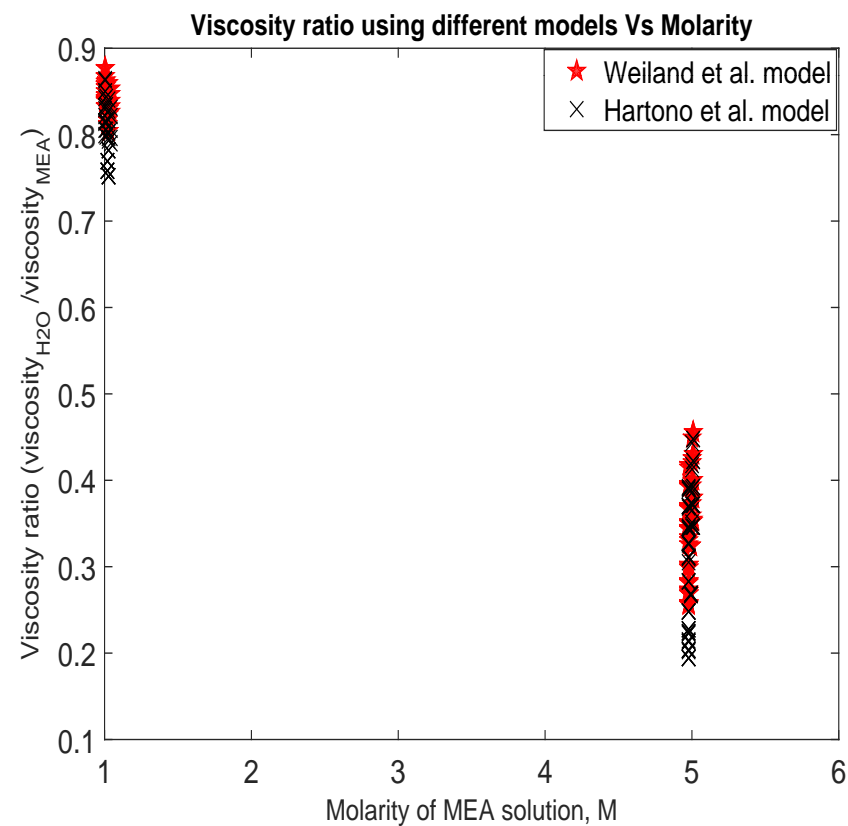
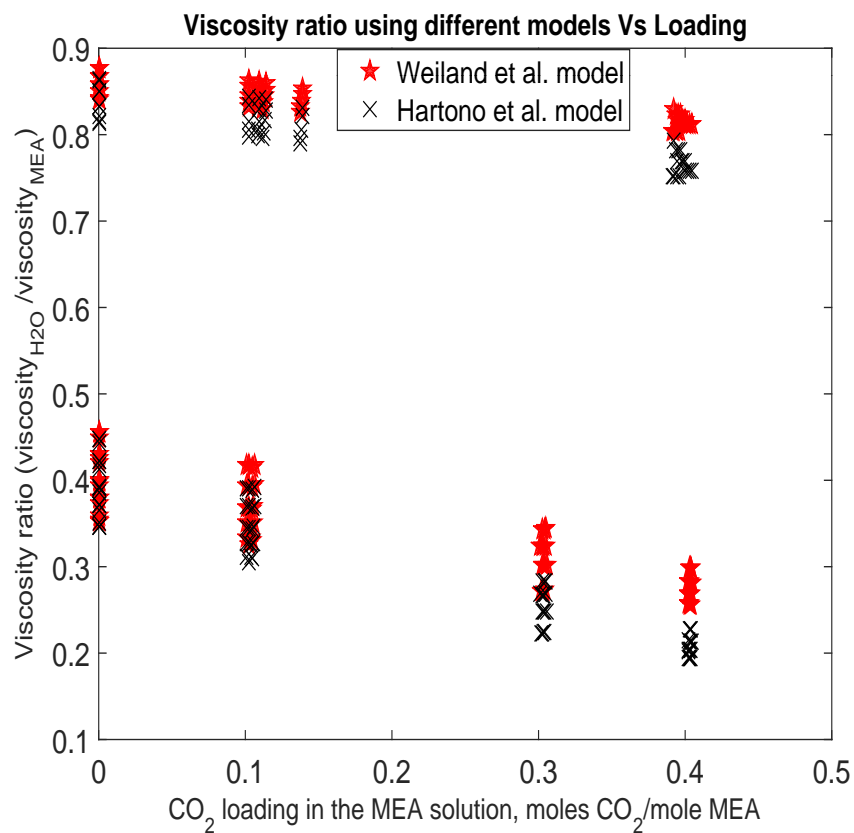


Case 3: Effect of using different viscosity correlations

Case 3	
Property	Source
Thermodynamic model	Inhouse e-NRTL model
Kinetic model	Inhouse
$D_{CO_2_MEA}$	Ko et al. (2000)
D_{MEA_MEA}	Snijder et al. (1993)
Viscosity	Hartono et al. (2014)

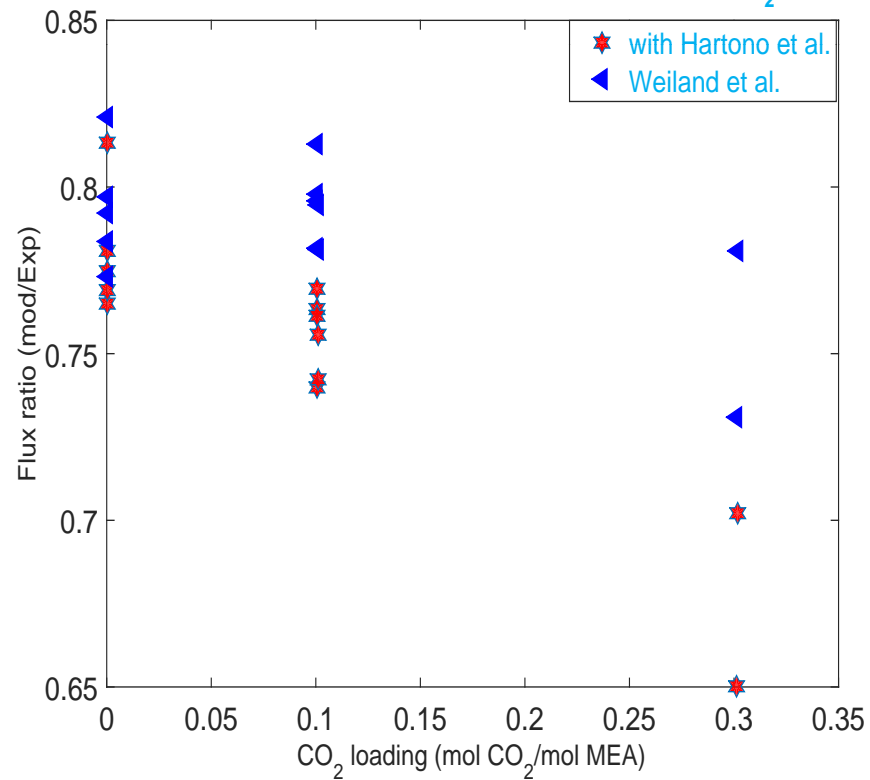
Viscosity correlation changed to **Weiland et al. model(1998)**

How different are these viscosity correlations??

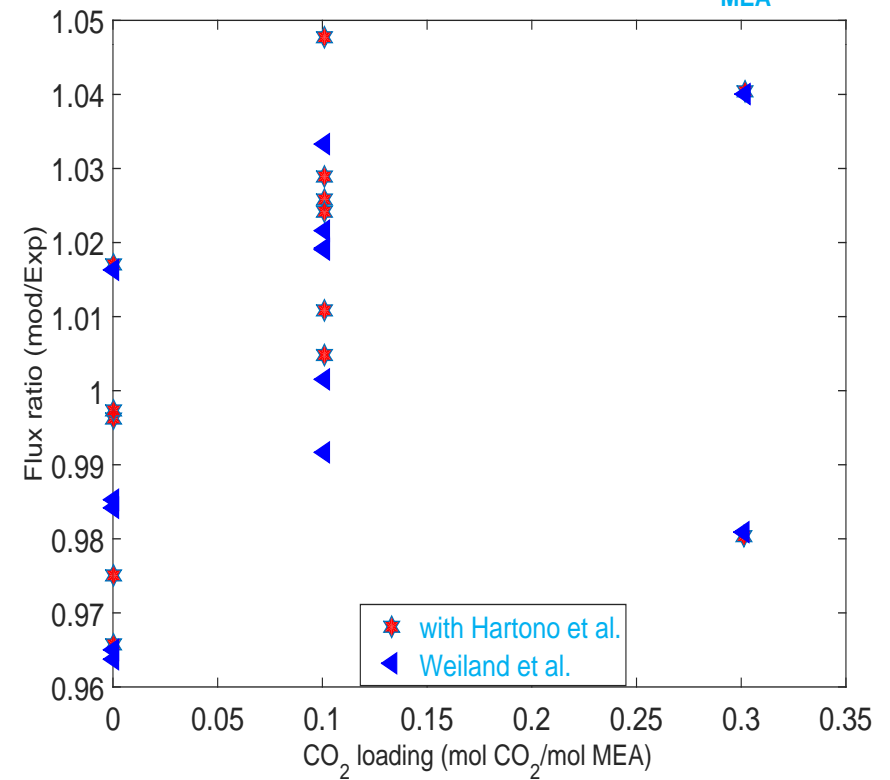


Results : Case 3

Viscosity correlations in Versteeg et al. D_{CO_2}



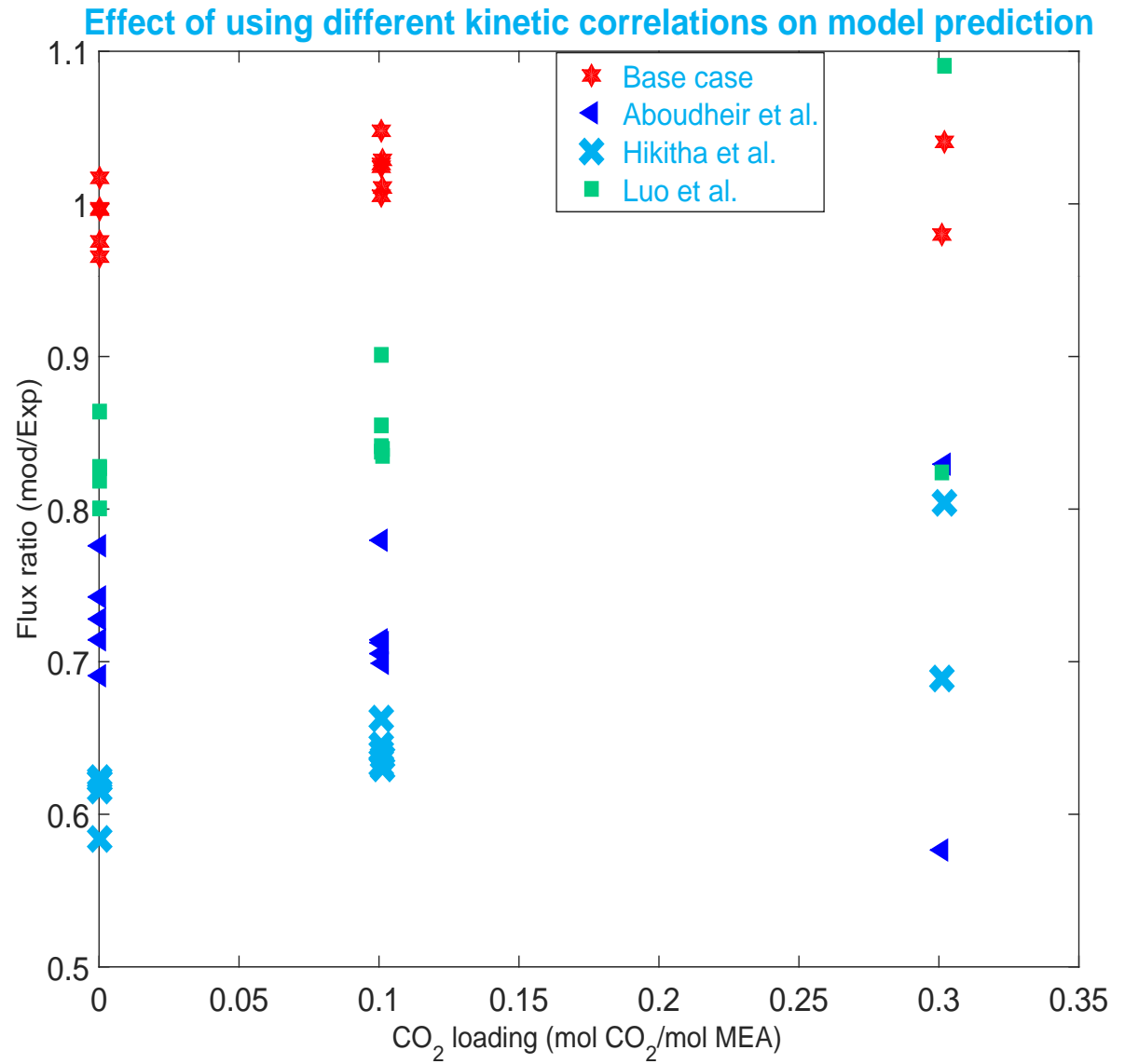
Viscosity correlations in Snijder et al. D_{MEA}



Case 4: Effect of using kinetic constants correlations

Case 4	
Property	Source
Thermodynamic model	Inhouse e-NRTL model
Kinetic constants correlations changed to Aboudhair et al. (2003) , Hikitha et al. (1977) & Luo et al. (2015)	
$D_{CO_2_MEA}$	Ko et al. (2000)
D_{MEA_MEA}	Snijder et al. (1993)
Viscosity	Hartono et al. (2014)

Results : Case 4

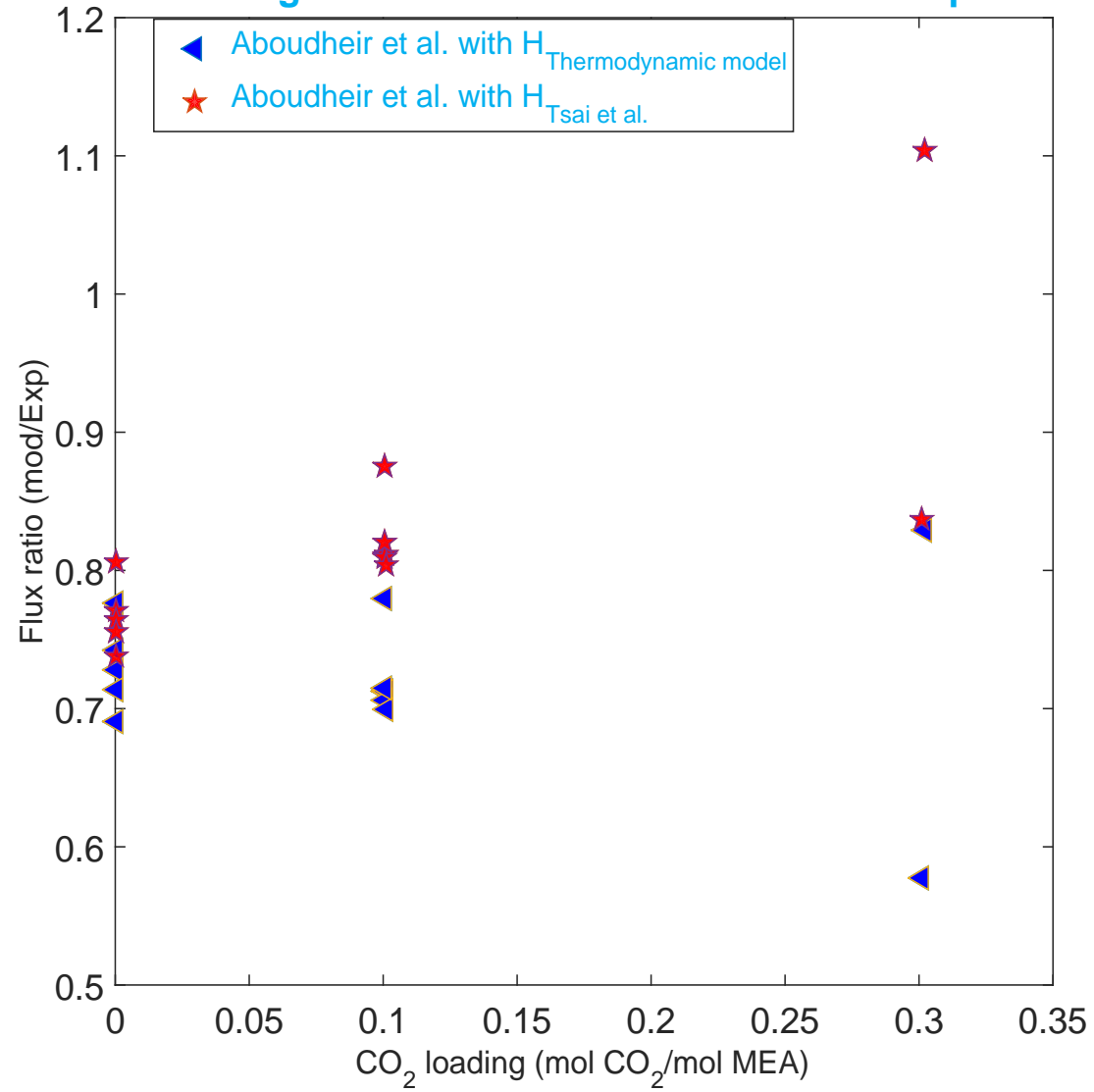


Case 5: same set of correlations/ correct combination

Case 5	
Property	Source
Thermodynamic model	Inhouse e-NRTL model + Tsai et al. (2000) (Henry's constant)
Kinetic model	Aboudheir et al. (2003)
$D_{\text{CO}_2\text{-MEA}}$	Ko et al. (2000)
$D_{\text{MEA-MEA}}$	Snijder et al. (1993)
Viscosity	Weiland et al. (1998)

Case 5

Effect of using same set of correlations on model prediction



Conclusions

- It's very important to use correct set of correlations in model to represent the data
- If possible, use complete set of correlations used in the model development
 - Especially in sensitivity studies and scale up
- Henry's law constant and diffusivity of CO₂ in MEA, kinetics have high sensitivity in the model
- With different combinations of parameter correlations, model gives different predictions for the same case



