CO_2 Removal using a Synthetic Analogue of Carbonic Anhydrase

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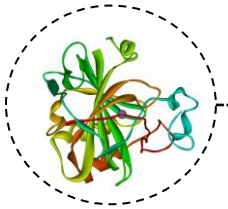
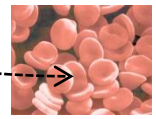
WorleyParsons
resources & energy

GL Chemtec International

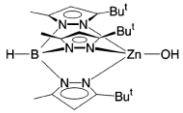
CO_2 Capture with Enzyme Synthetic Analogue



Carbonic anhydrase

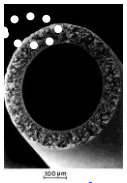


Erythrocytes (red blood cells)



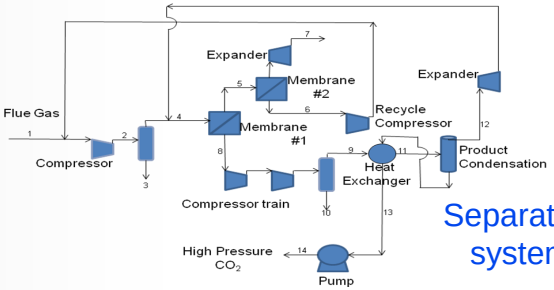
Carbonic anhydrase Synthetic analogue

CO_2 -Selective film

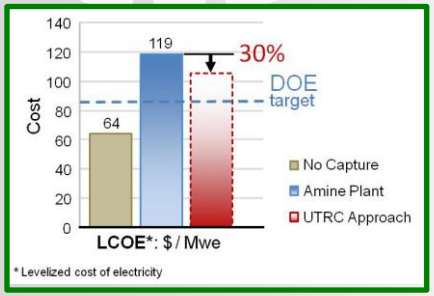


Porous substrate

Membrane module



Separation system



2010

Membrane prop. mapping

Atomistic model verification

≥3 paths to films

No unrecoverable poisoning

Q1 | Q2 | Q3 | Q4

2011

Three model films prepared

Selectivity improvement demonstration

≥100 selectivity ≥ permeance

30% cost reduction vs. amines

Q1 | Q2 | Q3 | Q4

≥200 hr durability test

▲ : Accomplished △ : Pending △ : Go / No go

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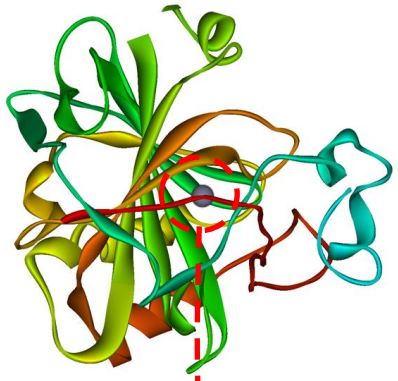
Carbonic Anhydrase: Nature's Solution

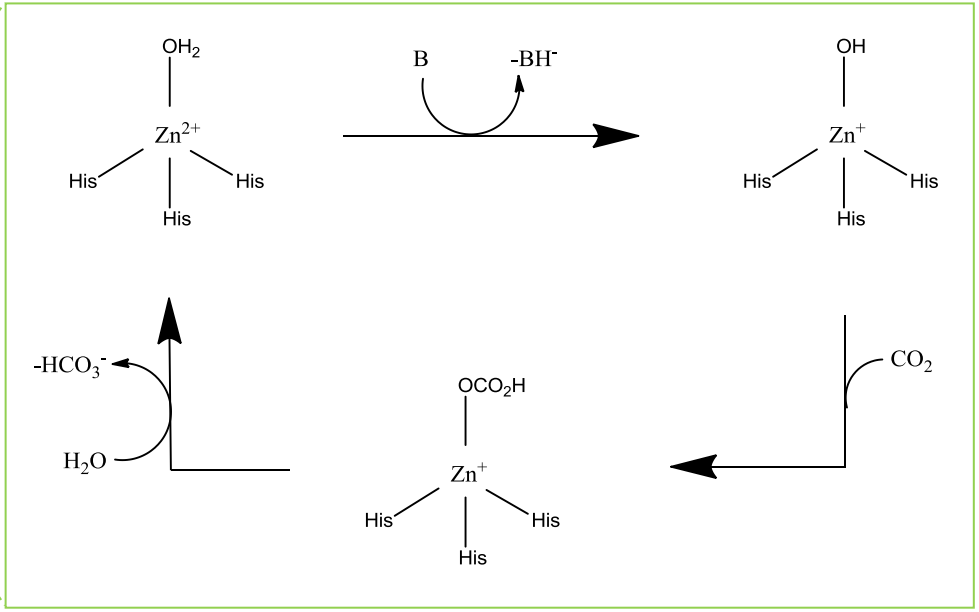
What we can learn from the enzyme: reactive, coordinated ZnOH site

Active site's fast, reversible interaction with CO_2

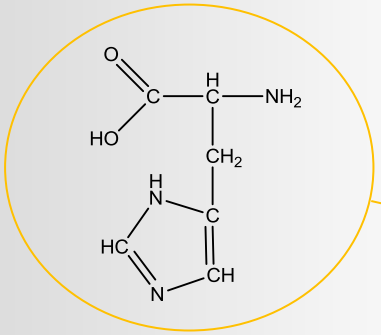
Carbonic anhydrase

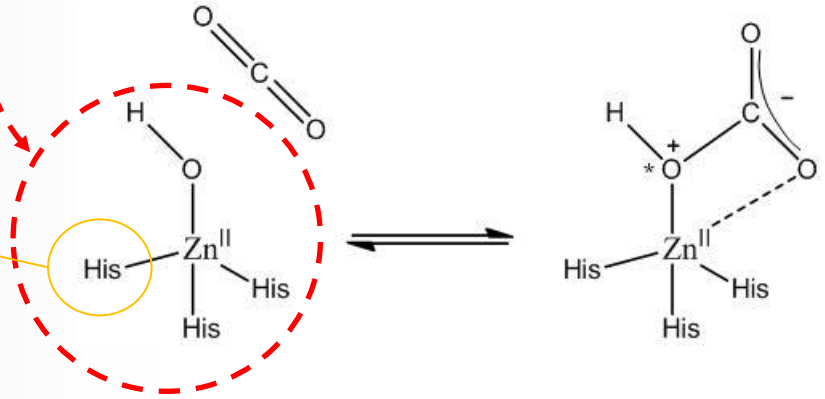
Red blood cells





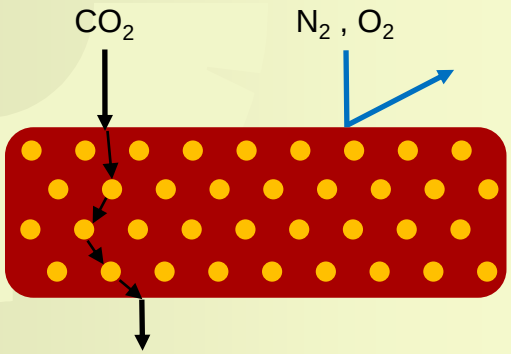
Histidine
(an amino acid)





Proposed Approach: Membrane-based Separation

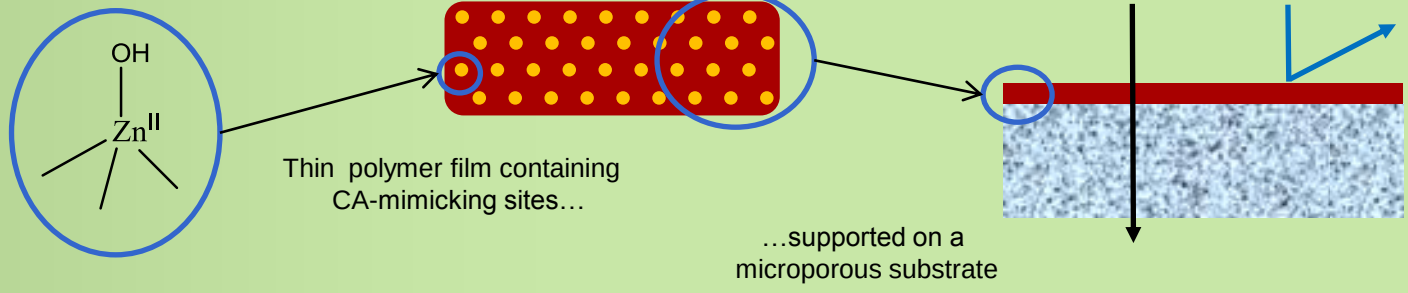
CO_2 transport facilitated by carriers mimicking enzyme active site



"Ideal" membrane:

- CO_2 transport is facilitated by specialized "carriers" within a barrier film
- Requires sites exhibiting fast and reversible interaction with CO_2

Proposed approach:



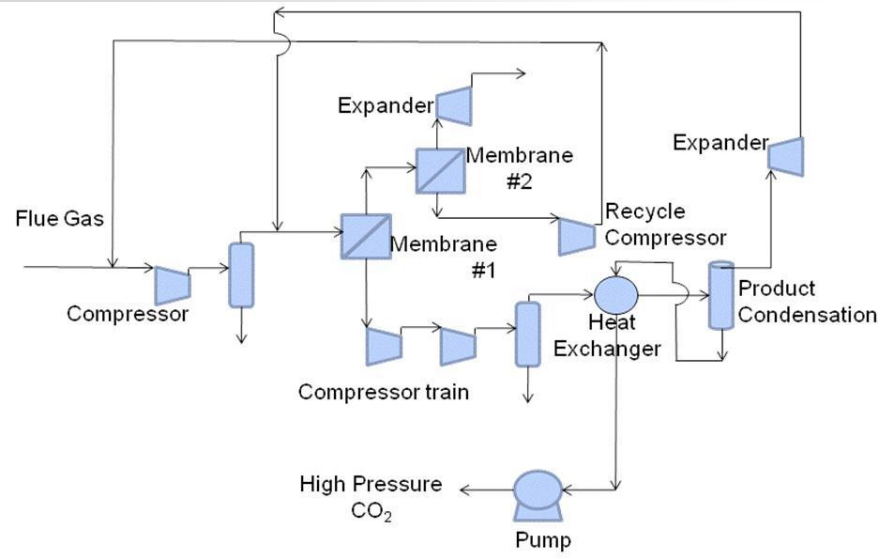
- ~30% lower CO_2 capture cost compared to liquid amines
- ~2 billion tons/yr CO_2 from existing coal-fired power plants
- Modular, skid-mounted configurations; no moving parts
- Flexibility to start with smaller system, gradually increase to 90% CO_2 capture

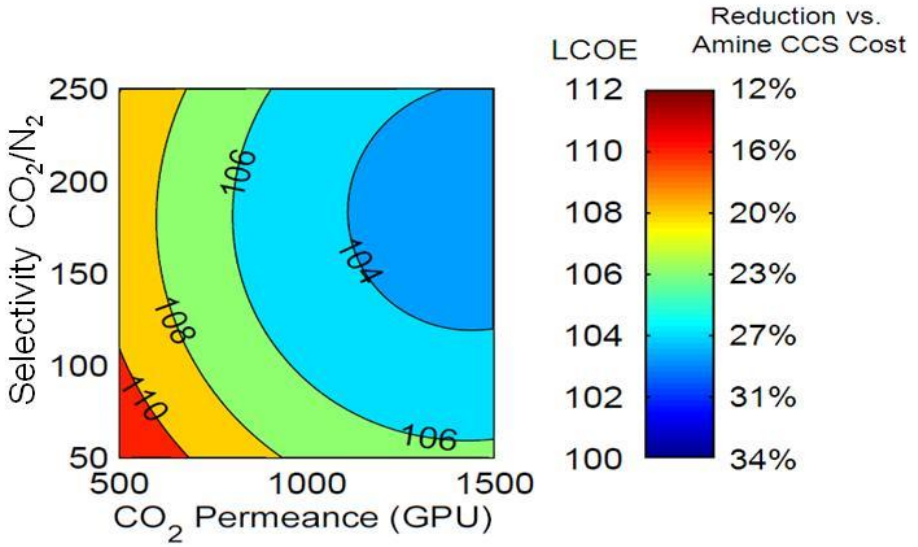
Q1 Milestone: Separation System Simulation

Accomplishment

Q1 Milestone (3/31/2010):

A membrane-based separation system simulation model in Aspen HYSYS® will have been completed and audited by WorleyParsons for independent assurance that plant interface conditions have been captured appropriately; and system sensitivity to membrane selectivity and permeance will have been mapped.





Simulated separation system (simplified) → Membrane properties mapping

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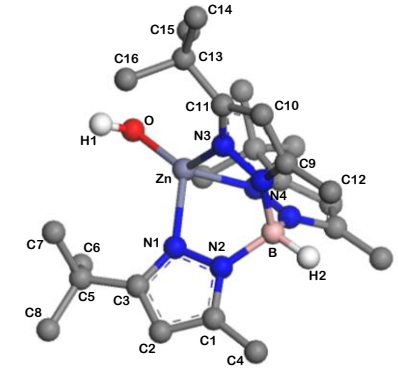
Q2 Milestone: Atomistic Modeling

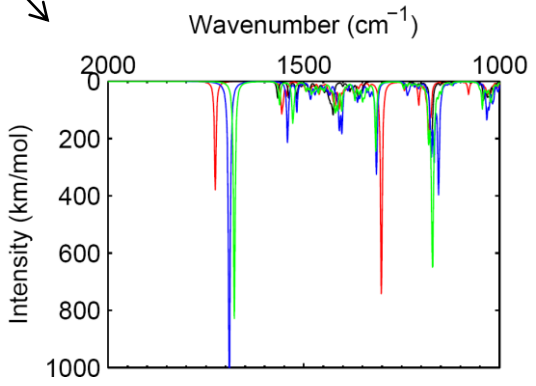
Accomplishment

Q2 Milestone (6/30/2010):

Atomistic level model of synthetic analogue in DMol^3 ® will have been completed and its ability to predict the bicarbonate derivative identified by NMR will have been demonstrated.

- Calculated structure predicts bond lengths & angles observed experimentally (XRD)
- Similar IR bicarbonate peaks observed in simulations and experiments
- Reasonable comparison between experimental and calculated analogue NMR



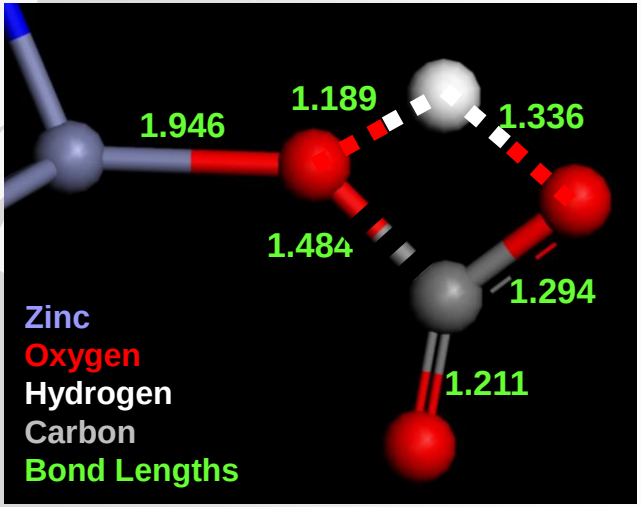


^{1}H

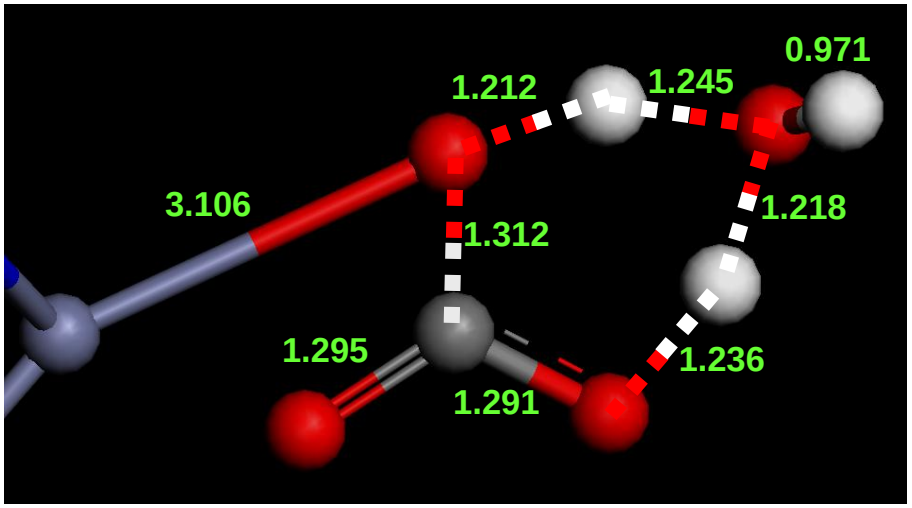
Atom	Vacuum	Chloroform	Benzene	Experimental
H1	-1.0	-0.7	-0.8	-0.3
H2	4.8	4.8	4.8	*
H(C2)	5.8	6.0	5.9	5.7
H(C4)	2.5	2.6	2.6	2.1
H(C6)	1.5	1.4	1.5	1.6

Insight from Atomistic Model

DMol³ predicts low E_A in the presence of water – similar to carbonic anhydrase



Zn
O
C
H
N
B



Explicit Molecule	Dielectric Solvent	E_A (kcal/mol)	ΔH_{rxn} (kcal/mol)
None	None	24.8	-7.0
None	Water	22.4	-8.5
None	Benzene	24.0	-4.1
Water	None	-0.2	-8.0
Water	Water	1.1	-8.2

- Significant change in reactive barrier with the participation of water molecules
- Small amounts of water in benzene/chloroform may provide sufficient catalysis effects
- Synthetic analogue predicted to mimic CA in aqueous environment (currently not our approach)

Next Steps: Test Resistance to Flue Gas Contaminants

Demonstrate no unrecoverable analogue poisoning (go/no go milestone)

Concentrations over membrane calculated from HYSYS® model

Max concentrations from WorleyParsons data (Sub-bituminus, bituminous A / B /C & lignite A / B

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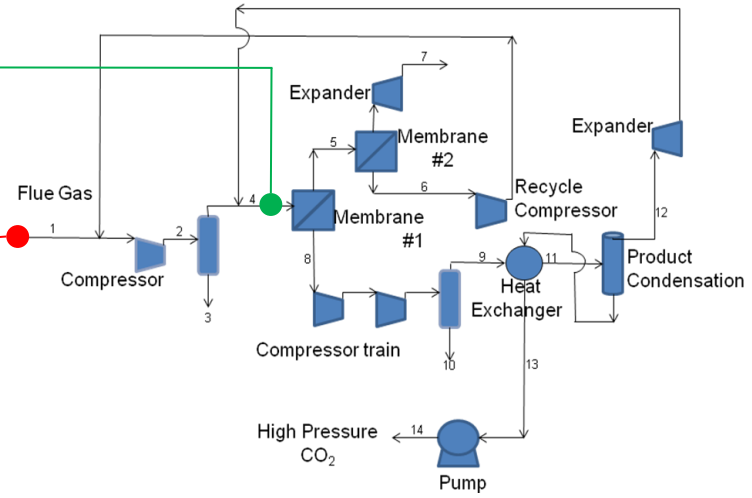
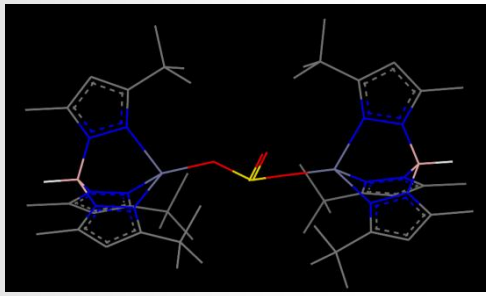
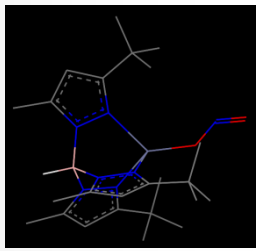


Example possible structures (predicted by DMol^3)





?

?

	mol %
Water	1.70
Oxygen	2.83
Nitrogen	78.61
Argon	0.94
CO_2	15.92
HCl	0.00115287
SO_2	0.00430116
SO_3	0.00004346
NO_2	0.00035149
HF	0.00005983