

MOLECULAR DYNAMIC SIMULATION OF
AMINE-BASED ABSORPTION PROCESS
FOR CO₂ CAPTURE

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STUDENT'S DECLARATION

I hereby declare that the work in this thesis is based on my original work except for quotations and citations which have been duly acknowledged. I also declare that it has not been previously or concurrently submitted for any other degree at Universiti Malaysia Pahang or any other institutions.

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“I write to give myself strength. I write to be the characters that I am not. I write to explore all the things I’m afraid of”

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LIST OF SYMBOLS

α_i	Acceleration
Å	Amstrong
N_i	Atomic Population
r_i	Change In Particle Position
ρ	Density
E	Energy
fs	Femtosecond
f_i	Force Of Newton's Second Law Of Motion
K	Harmonic Force Constant
m_i	Mass Of Particle
μm	Micrometer
ns	Nanosecond
N	Number Of Mole
U_{AB}	Potential Energy
P	Pressure
r	Spherical Radius
T	Temperature
K_{Ga}	Volumetric Mass Transfer Coefficient
V	Volume
wt.%	Weight Percent
∇_i	3-Dimensions

LIST OF ABBREVIATIONS

AMP	2-Amino-2-Methyl-1-Propanol
AMPCOO ⁻	2-Amino-2-Methyl-1-Propanol Carbamate
CO	Carbon Monoxide
CH ₄	Methane
CO ₂	Carbon Dioxide
CCS	Carbon Capture And Sequestration
CFBC	Circulating Fluidized Bed Combustion
COSMO- RS model	Conductor-Like Screening Model For Realistic Solvents
DFT	Density Functional Theory
DMEA	N,N-Dimethylethanolamine
DEEA	N,N-Diethylethanolamine
DMAEOE	2-[2-(Dimethylamino) Ethanoxy] Ethanol)
H ₂ S	Hydrogen Sulfide
H ₂ O	Water
H ₂ CO ₃	Carbonic Acid
HCO ₃ ⁻	Bicarbonate Ion
HMDA	Hexamethylenediamine
ID	Inside Diameter
IBC	Isolated Boundary Condition
IGCC	Integrated Gasification Combined Cycle
IL	Ionic Liquid
LiF	Lithium Fluoride
MEA	Monoethanolamine
MEACOO ⁻	Monoethanolamine Carbamate
MM	Molecular Mechanic
MD	Molecular Dynamic
MDEA	Methyl-Diethanolamine
MIPA	Monoisopropanolamine
MgCl ₂	Magnesium Chloride
MgSO ₄	Magnesium Sulfate

MSD	Mean Square Displacement
NaCl	Sodium Chloride
NMP	Normal Methyl Pyrrolidone
NH ₃	Ammonia Compound
O ₂	Oxygen
RDF	Radial Distribution Function
PBC	Periodic Boundary Condition
PC	Propylene Carbonate
PSA	Pressure Swing Adsorption
PZ	Piperazine
PZH ⁺	Protonated Ion Of PZ
PZEA	(Piperazinyl-1)-2-Ethylamine
PZCOO-	Piperazine Carbamate
PCM	Polarizable Continuum Model
SiO ₂	Silicon Oxide
TEA	Triethanolamine
TBP	Tributyl Phosphate
TSA	Temperature Swing Adsorption
VAC	Velocity Autocorrelation
WWC	Wetted Wall Column
3DMAP	3-Dimethylamino-1-Propanol
1DMA2P	1-Dimethylamino-2-Propanol
¹³ C NMR	Carbon-13 Nuclear Magnetic Resonance
-OH	Hydroxyl Group
-NH	Amino Group