MOLECULAR DYNAMIC SIMULATION OF AMINE-BASED ABSORPTION PROCESS FOR CO_2 CAPTURE

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SUPERVISOR'S DECLARATION

I hereby declare that I have checked this thesis and in my opinion, this thesis is adequate in terms of scope and quality for the award of the degree of Master of Engineering in Chemical

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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_2S	Hydrogen Sulfide
H_2O	Water
H_2CO_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
NaCI	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