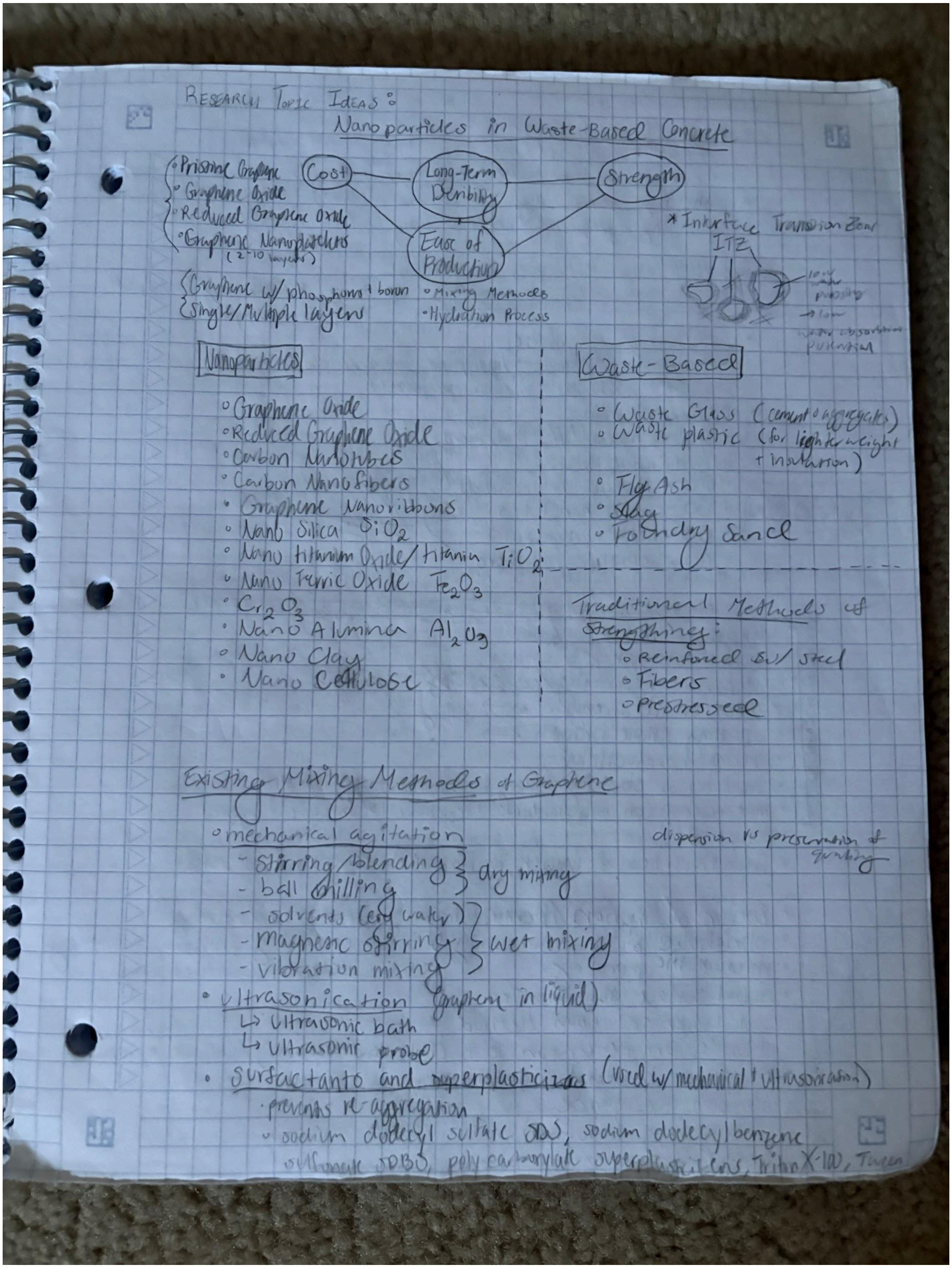
First starting out, I was exploring blended cement with nanoparticles, specifically hybrids of nanomaterials, different mixing methods, and different methods to prevent graphene agglomeration.



RESEARCH TOPIC IDEAS:

Nanoparticles in Waste-Based Concrete

- Pristine Graphene
- Graphene Oxide
- Reduced Graphene Oxide
- Graphene Nanoplatelets (2-10 layers)

Graphene w/ phosphorus + boron
Single/Multiple layers

Cost — Long-Term Durability — Strength — Ease of Production

- Mixing Methods
- Hydration Process

* Interface Transition Zone
ITZ

Nanoparticles

- Graphene Oxide
- Reduced Graphene Oxide
- Carbon Nanotubes
- Carbon Nanofibers
- Graphene Nanoribbons
- Nano Silica SiO_2
- Nano titanium Oxide/titania TiO_2
- Nano Ferric Oxide Fe_2O_3
- Cr_2O_3
- Nano Alumina Al_2O_3
- Nano Clay
- Nano Cellulose

Waste-Based

- Waste Glass (cement & aggregates)
- Waste plastic (for lighter weight + insulation)
- Fly Ash
- Slag
- Foundry Sand

Traditional Methods of Strengthening:

- Reinforced w/ steel
- Fibers
- Prestressed

Existing Mixing Methods of Graphene

- mechanical agitation
  - stirring/blending } dry mixing
  - ball milling
  - solvents (e.g. water) } wet mixing
  - magnetic stirring
  - vibration mixing
- ultrasonication (graphene in liquid)
  - ↳ ultrasonic bath
  - ↳ ultrasonic probe
- surfactants and superplasticizers (used w/ mechanical + ultrasonication)
  - prevents re-aggregation
  - sodium dodecyl sulfate SDS, sodium dodecylbenzene sulfonate SDBS, polycarboxylate superplasticizers, Triton X-100, Tween

dispersion vs preservation of graphene

- high shear mixing
  - powerful mechanical forces
  - use of rotor-stator mixers, homogenizers, ball mills
- planetary ball mixing (for ceramic matrices)
  - milling of graphene & ceramic using balls in rotating container

Surface Modification techniques for graphene
(to enhance compatibility w/ concrete)

★ Collab w/ concrete companies

- Oxidation of graphene
  - hydrophobic graphene → hydrophilic graphene oxide
  - reduces mechanical & conductive properties
- Polymer Grafting
  - grafting hydrophilic polymers
- nanomaterial hybrids
  - GO + inorganic nanomaterials
  - GO - carbon nanotubes
  - GO - silica nanoparticles
  - GO - sepiolite nanofibers

} hybrid materials

$\boxed{\text{Nano } SiO_2@GO}$

~~graphene nanoplatelets~~ vs ~~functionalized graphene oxide~~

MECHANICAL PROPERTIES

- compressive strength ~~(0.05)~~
- flexural strength bending
- electrical resistivity/conductivity
- direct tensile strength ⟷ pulling
- splitting tensile strength ⟷
- thermal conductivity
- modulus of elasticity - (tendency to deform elastically) high = stiff
- more research on microhardness, & resistance to fracture & impact

- Fresh Properties of Concrete vs Hardened Properties of Concrete

DURABILITY / LONG TERM

- Water absorption / permeability
- shrinkage
- micrometric porosity
- Initial Surface Absorption Test
- Boil Water Saturation Method
- Chloride Ion Penetration Test (Chloride Penetration) / Chloride Ingress Resistance
- Resistance to Acid & Sulphate
- Abrasion Resistance
- Workability (slumps)
- Thermal Diffusivity

- water sorptivity
- mercury Intrusion Porosimetry
- Thermal Conductivity

- Chemical Resistance/Corrosion Protection
  - ↳ graphene preventing metal oxidation
- Freeze-thaw Resistance (graphene indirectly affects thaw process)
  - GO + Fly Ash to Steel fiber reinforced concrete
  - GO + silica fume
- Fire Resistance

ELECTRICITY/THERMAL

- Electrical Conductivity
- Thermal Diffusivity
  - GO's functional groups = high conductivity
  - graphene nanoribbons ↗
  - GO is electrically insulating b/ of oxygen functionalities →
    GO reduction = increased conductivity

- model that predicts crack propagation behavior of cement mortar w/ graphene oxide
- graphene promotes hydration process
- GO + Fly Ash offset negative effects of environment
- sulfonated graphene nanosheets delay dissolution & induction of Calcium silicate (C_3S) + hinder hydration reaction

GO improves mechanical properties + microstructure of ITZ of recycled concrete
Graphene + ITZ more research

Limitations of Graphene in Concrete

- decreased workability
- dispersion issues
- compatibility issues
- long term durability
- cost
- safety

graphene reduces concrete volume by 15% during hardening

Environmental Impacts

☆ Life Cycle Assessment LCA ☆

- concrete manufacturing → CO_2 emissions
- high energy consumption, water & resource consumption
  - ↳ use renewable energy
  - ↳ recycling solvents + reactants
  - ↳ waste recycling
  - ↳ recycled aggregates
  - ↳ bio-based binders
  - ↳ recycling
  - ↳ graphene concrete = hazardous waste → waste management
    - research environmental effects

I explored ideas involving limiting concrete's carbon footprint and increasing durability with nanomaterials, as well as decreasing the cost of nanomaterials in concrete.

Economic Viability

Graphene powder or Graphene-reinforced fibers to cement

Graphene Nanoplatelets + nanofibers

[CVD graphene = high quality + expensive
[Exfoliated Graphite = reaggregation + cheaper
↳ additional surfactants

High Shear Mixing + Ultrasonication
↳ adds to costs

More durable

- saltwater corrosion resistance / freeze-thaw resistance
- Silica Nanoparticles reduced calcium leaching (durable)
- Carbon Nanotubes

Recycled Aggregates w/ GO nanomaterials in cement
- problems w/ compatibility + performance

Using waste biomass as raw material for graphene production mitigates environmental impacts

[GO + Fly Ash
[GO + Silica Fume

★ [When is cost of graphene concrete justified?

$\pi \approx 3.3$

Cylinders (6in × 12in, 4in × 8in) — diameter, height

Cubes (6in × 6in × 6in, 4in × 4in × 4in)

diameter ≥ 3× nominal maximum size of course aggregate

$\underbrace{378in^3, 112in^3}_{\text{cylinders}}$, $\underbrace{216in^3, 64in^3}_{\text{cubes}}$

2%: $7.56in^3$, $2.24in^3$, $4.32in^3$, $1.28in^3$

Nanoparticles: $/g

GO: \$75-\$500

Reduced GO: \$190-\$200

Carbon Nanotubes: \$100-\$1000

Carbon Nano Fibers: \$3.8

Graphene Nanoribbons: very

Nano-
- SiO_2: \$0.23-\$3
- TiO_2 - \$0.5-\$2
- Fe_2O_3 - \$0.7-\$2
- Cr_2O_3 - \$2.6-\$12.6
- Al_2O_3 - \$0.2-\$0.7

Nano Clay - \$0.1-\$5

Nano cellulose - \$3-\$25

Concrete = $2400 \frac{kg}{m^3}$ = $0.081-0.087\ g/in^3$

$112in^3 \rightarrow 8.96g$

$216in^3 \rightarrow 17.28g$

$64in^3 \rightarrow 3.12g$

$378in^3 \rightarrow 30.24g$

2%: 6g, 1.8g, 3.5g, 1g

I worked out the cost to test my ideas physically, adhering to ASTM standards of testing.

Call w/ Jennifer Mitchel

ASTM C33 · ACI C94 ~~[illegible]~~

- blue planet systems – composition → aggregates (carbon capture)
  - in sf airport
  - ↳ Los Gatos
- US Concrete / central concrete – San Jose
  - ↳ recycled aggregates
  - ↳ more extensive lab
- produces → Carbon Cure

Johnny Alanen → expert (works with Jennifer's husband)

- Go to ~~her~~ Jennifer's LinkedIn
- NMRA – nonprofit, RA – (there's a company in Chicago)
- Meg Calkins – Prof. Landscape Sustainable concrete/materials
- Create LinkedIn
- actual concrete mix → fly ash, slag → strong
  - psi → pore surface reaction
- DESIGN:
  1) identify requirements (psi w/ "aggregate)
     - water-to-cement ratio
     - chemical admixtures for slumps (temperature)
  2) Formulas
     - specific gravity relative to water → gives lbs of thing
       - ↳ then calc. volume of each
  - different cements, different aggregate, different flyash

ZOOM: Thursday – 3 pm or 6 pm

I was able to call Jennifer Mitchel who was designing fire-resistant concrete about my ideas.

~~ASR - Alkali Silica Reaction~~
~~Alkalis + silica in aggregates~~

Alkali Modulus = Silica to Alkali ~~($SiO_2 : Na_2O$)~~
($SiO_2 : Na_2O$) ↖ activator

- higher = more silica = denser = improved workability
- lower = slow reactions

Alkali modulus, alkali admixture, water-binder ratio, fly ash admixture
Gypsum protects against sulfate attacks

Strengths of Geopolymer:
- workability
- compressive S.
- resistance to sulfates/acids
- ~~decreased~~ temp resistance
- decreased drying shrinkage + creep

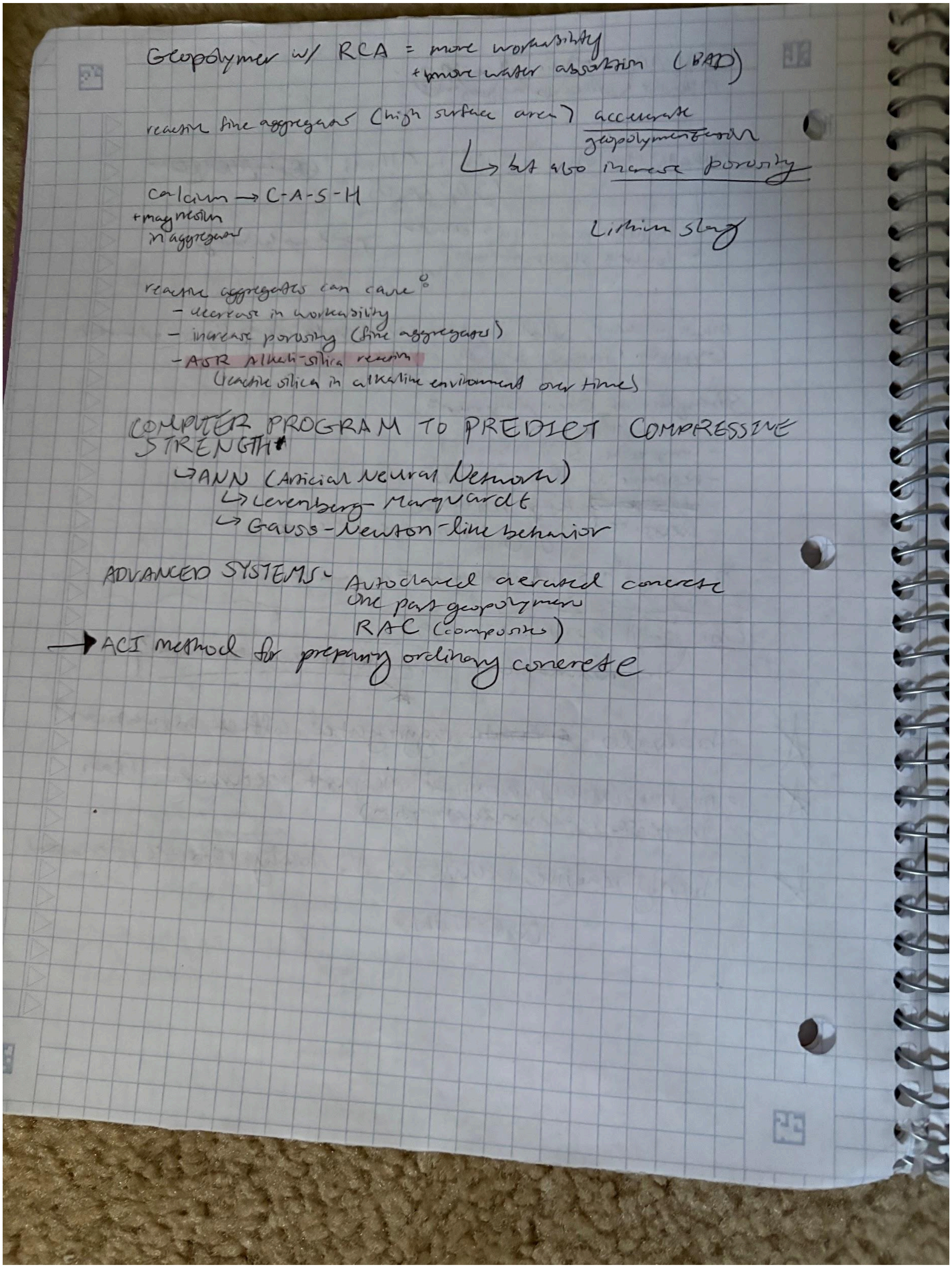
Precursor + solid activator ≠ in particle size

One part vs two part

One part ← less activated → how to increase reaction?

- ☆ how do ~~concrete~~ aggregates affect activation?
- ☆ mechanical activation of one part precursors (can increase reaction/activation)
- ☆ highly reactive precursors VS lowly reactive precursors
- QUESTIONS

I began exploring geopolymer concrete. I was very drawn to questions involving one-part vs two-part geopolymer concrete.



Geopolymer w/ RCA = more workability
+ more water absorption (BAD)

reactive fine aggregates (high surface area) accelerate geopolymerization
↳ but also increase porosity

calcium → C-A-S-H
+ magnesium
in aggregates

Lithium slag

reactive aggregates can cause:
- decrease in workability
- increase porosity (fine aggregates)
- ASR alkali-silica reaction
(reactive silica in alkaline environment over time)

COMPUTER PROGRAM TO PREDICT COMPRESSIVE STRENGTH*
↳ ANN (Artificial Neural Network)
↳ Levenberg-Marquardt
↳ Gauss-Newton-like behavior

ADVANCED SYSTEMS - Autoclaved aerated concrete
One part geopolymers
RAC (composites)

→ ACI method for preparing ordinary concrete

I also explored using recycled concrete aggregates in geopolymer concrete as well as beginning to think about predictive AI in concrete mix design.

→ Aggregates:

- Limestone (strong ITZ bond) VS Quartz (weak)
- Al-O-Si + hydrogen bonding between geopolymer + silica aggregate = strong ITZ
- Recycled ceramic aggregate
- Elemental Concentrations of geopolymer change when aggregates change
- Fine aggregates → surface dissolution in highly alkaline geopolymer → releases Si → motivates geopolymer
- Aggregates on ITZ
- Alkaline environment → aggregates more influential

→ Setting Time:

- Fast setting time → need more workability

Accelerate Setting:

- more calcium (fa & ggbs)
- more alkaline activator
- increase Si/Al ratio : (more silica)
- heat curing

Delay Setting:

- chemical retarders (borax, sodium gluconate, sucrose)
- reduce fly ash (class F) & reduce slag
- increase water-solids ratio : more water
- type & concentration of activator
  - higher sodium silicate reduces setting time

I researched key features of geopolymer concrete and brainstormed any questions/thoughts that popped up.

Workability
- use well-grade aggregates (avoid voids)
- add fine particles of FA, silica fume, ggbs (reduce friction)
- ratio of sodium silicate/sodium hydroxide
- superplasticizers
- increase water-to-solid ratio
- retarders
- avoid reactive fly ash
- water → increased porosity during heat curing

SHRinkage
- decrease water/solid ratios - less water = less shrinkage
- ggbs/microsilica can lessen shrinkage
- chemical additives to reduce shrinkage:
  - superabsorbent polymers SAPs
  - expansive agents & shrinkage-reducing admixtures
    EAs SRAs
  - magnesium & calcium oxides
- increase temp & humidity during curing
- lightweight aggregates / internal curing agents
  → retains moisture & reduces capillary pressure
- increase aggregate/binder ratio
- water reducing agents to control water content & improve workability

Mitigating efflorescence:
- low alkali content OR Alkali/Alumina ratio
- less water
- admixtures: plasticizing/compaction aid, waterproofing admixture

Chemical Resistance
- precursor, alkali activator (influence geopolymerization)
- calcium → decalcified
- precursors w/ silica
- sodium metasilicate + sodium hydroxide less resistant than sodium aluminate & sodium carbonate
- N-A-S-H very important

GEOPOLYMERIZATION IN ONE-PART

- one reaction is more difficult to control than two separate
- hydration:
  - heat emits
  - depends on activator
  - kinetics not understood b/c it varies alot
  - different raw materials make it hard to predict in one-part
- flash setting
- <u>using multiple activators</u>
- pore structure in one part

ACI standards ⟶ (onepart) geopolymer ?

predictive models? mix design? some sort of engineering?

I began questioning the lack of standards for geopolymer concrete.

MODELS:

ResNet + XGB > BPNN, ANFIS, RF, DT, ANN

ANFIS > ANN, GEP

DT + RF > K-Nearest Neighbors

MEP > GEP

ANN > GEP

ANFIS > ANN

GPR > LR, SVM, EL, ANN

ANN-LM > ANN-GA, ANN-PSO

GEP > MEP

ANN > GP, EPR

GP-RF >

DNN > KNN, SVM

XGB > DT, RF

XGB > SVM, MLP

ANN > RF, XGB

DNN > ANN, CNN

GB (Gradient Boost) > RF, XGB

With Sparrow Search Algorithm → XGB > BPNN, SVR, RFR, GBR, lightGBM

GMDH-NN + KNN > GSVR, DT, RF, XGB

GB + KNN

SVM > BPNN, ELM

RFR > KNN, LR

I recorded the results of studies determining the most accurate model for predicting geopolymer concrete properties.

~~Boost~~

ResNet
- neural network
- deep learning

XGBoost
- ensemble model
- multiple decision trees
- regression and classification
- optimizes regularization, handling missing data, + using hardware resourses (unlike normal boosting)

Back-Propagation Neural Network
- neural network
- error back-propagation algorithm
- strong non liner mapping

Adaptive Neuro-Fuzzy Inference System
- ANN + Fuzzy Logic
- interpretable + complex, nonlinear functions

Random Forest
- supervised
- ensemble learning model
- multiple descion trees
- classification and regression

Decision Tree
- supervised
- classification + regression

ANN
- non parametric
- complex patterns

~~Gene Expression Programming~~
- ~~evolutionary algorithm~~

~~Multi-Expression Programming~~
- ~~evolutionary algorithm~~

K-Nearest Neighbors
- non parametric
- supervised
- classification + regression

I compared different AI models.

models

- Neural Networks - commonly used for various tasks b/c they learn complex patterns from large datasets
- Linear Regression - identifies correlations between variables
- Support Vector Machines - classification
- Decision Trees - splits data into branches based on feature values (classification)
- K-means clustering - sorts data based on similarity (discovers underlying patterns)

→ Unsupervised learning - no guidance, unlabeled data

~~Types~~ Algorithms:

- Clustering
- Dimensionality Reduction
  - ↳ Noise Reduction
  - ↳ Data Visualization

} common tasks

→ Supervised Learning - labeled data, data annotation

Types of Algorithms:

- Regression
- Classification
- Forecasting

You can combine these algorithms (ex: unsupervised dimensionality reduction + supervised regression)

→ Reinforced ML Algorithms - trains within environment w/ rules + goal (ex: chess, driving)

- Unsupervised Dimensionality Reduction
- Supervised Regression
- Simple or Esemble methods (combine models)
  - random forests, gradient boosting, XGBoost
  - ↳ linear regression, decision trees, k-means clustering

- simple more interpretable; descion tree-based esmemble methods like random forests = good trade off

Gaussian Process Regression
- non parametric
- Gaussian Process
- Complex, non-linear relationships

Support Vector Machine
- classical (not deep learning)
- classification & regression

~~Genetic Programming + Evolutionary Polynomial Regression~~

Multilayer Perceptron
- neural network
- deep learning
- classification, prediction, pattern recognition

Gradient Boosting
- multiple decision trees
- ensemble method
- sequential training (unlike random forests
- classification & regression

Light Gradient Boosting Machine
- speed + efficiency
- algorithm = Gradient Boosting Decision Tree
- large datasets & high-dimensional data
- supervised

Group Method of Data Handling Neural Network
- self organizing
- polynomial regression

Generalized Support Vector Regression
- nonlinear
- support vector Regression
- apply SVM elsewhere

Extreme Learning Machine
- neural network
- no backpropagation
- fast

shapley additive explanations SHAP
sensitivity + parametric analysis

Bayesian regularization algorithm
* Levenberg-Marquardt algorithm
scaled conjugate gradient algorithm

ANN

XGBOOST

Bayesian hyperparameter tuning technique
5-fold cross validation

Multi-objective Particle Swarm Optimization

Bayesian Optimization

Multi-objective optimization techniques
- Non-dominated sorting genetic algorithm II
- multi-objective particle swarm optimization
- genetic algorithm w/ fuzzy models

Hoffman + Gardener's sensitivity Analysis

I took notes on how others used and what they used with XGBoost to predict properties of geopolymer concrete.

INPUTS:

fly ash concentration
+ fineness

slag content

silica fume

cement content

magnesium oxide (MgO)

calcium oxide (CaO)

calcium hydroxide content ($Ca(OH)_2$)

calcium sulfate $CaSO_4$

sodium oxide content (Na_2O) {Not added, formed}

sodium hydroxide content ($NaOH$)

sodium silicate content (Na_2SiO_3) + ~~(Na_2Si)~~

plus Molarity

In 1 Part:
- Lithium hydroxide
- Potassium Carbonate

water/binder ratio or water/solid
(or just water)
+ ↳ water to solid ratio of fly ash

extra water

curing temp

coarse aggregate
→ ratio between two

fine aggregate

~~alccofine?~~ gravel (4/10mm + 10/20mm)

age

superplasticizer / admixture (HRWR eg)

heat curing days

Na/Al

Si/Al

precuring

the specific gravity of cement

I brainstormed a list of possible inputs based on studies.

INPUTS - COMPOSITIONS

silicon oxide content (SiO_2) } NOT ADDED FORMED }

aluminium oxide content (Al_2O_3)

iron (III) oxide content (Fe_2O_3)

metakaolin

~~hydroxide concentration~~

calcined clay, quarry stone dust, caustic soda, waterglass

SiO_2 / Na_2O

SiO_2 / Al_2O_3

Na_2O / Al_2O_3

H_2O / Na_2O

alkaline/activator binder

~~SiO_4 / OH~~ (silicate/hydroxide)

$Na_2SiO_3 / NaOH$

fly ash/binder

coarse aggregate / binder

fine aggregate / binder

water/ Fly Ash

coarse/ Fly Ash

fine/ fly Ash

molarity of activator

nano-TiO_2 / nano-SiO_2

fineness modulus of fine aggregate

max size of coarse aggregate

silica modulus (SiO_2 / ($Al_2O_3 + Fe_2O_3$))

$NaOH$ / ~~$NaOH$~~ Na_2SiO_3

fly ash/aggregate

activator/ fly ash

$\frac{NaOH + \text{sodium silicate}}{\text{fly ash}}$

Responses other than compressive Durability I Environmental II Workability IIII
~~Combination of precursors~~ (~~IIII IIII II~~)
bond strength (2 studies)
one part (2 accesible studies)

$\frac{Si}{Al}$, alkali activator type + concentration, curing temp, water content

GAPS:

- Outputs:
  - Durability (1 source)
  - ~~Environmental Impact (2 sources)~~
  - Workability (4 sources[5])
  - Bond strength (2 studies)
- 1 Part (2 sources)

*Need a lot of experimental data to create accurate AI model
(generally, most studies have 1000 datapoints (200-1000))

1 Part = easier to mix; safer mixing & storage
2 Part = more complete reaction; higher compressive strengths as opposed to 1 Part (faster setting time, less consistent reaction)

CHEMICAL DURABILITY

I determined the major gaps I was seeing in my initial research.

ASTM Standards

C 192 Standard Practice for Making and Curing Concrete Test Specimens in the Laboratory

~~C330 Specification for Lightweight aggregates for structural Concrete~~

C470 Specification for Molds for Forming Concrete Test Cylinders Vertically

C494 Specification for chemical admixtures for concrete

C511-21 Specification for Mixing Rooms, ~~Mixing~~ Moist Cabinets, Moist Rooms, and water storage tanks used in testing of Hydraulic Cements and concretes

C617 Practice for Capping Cylindrical concrete specimens

C1077 Practice for Laboratories testing Concrete and Concrete aggregates for use in construction and criteria for Lab evaluation

~~ACI 309 Guide for concrete Consolidation~~

C39 Standard Test Method for Compressive Strength of Cylindrical Concrete Specimens

C33 Standard Specification for Concrete Aggregates

C702? Standard Practice for Reducing samples of Aggregate to Testing size

~~C192~~ C114-24 Standard Test Methods for Chemical Analysis of Hydraulic Cement

C1005-20 Standard Specification for Reference Masses and Devices for Determining Mass and Volume for Use in Physical Testing of Hydraulic Cements

C1222-23 Standard Practice for Evaluation of Laboratories Testing Hydraulic Cement

C183 Standard practice for sampling and the amount of testing of hydraulic cement

In my initial search, I noted and read ASTM and ACI standards that may apply to my research.

C1451 - ~~24~~ Standard Practice for Determining Variability of Concrete-making materials from single source
+ 1451-05

C150 Standard Specification for portland Cement

~~C1074-19e1 Standard Practice for estimating con~~

C295 Standard Guide for Petrographic examination of aggregates for concrete

C294-24 Standard descriptive nomenclature for constituents of concrete aggregates

C856 Standard practice for petrographic examination of hardened concrete

~~C1723-25 Standard Guide for examination of hardened concrete using scanning electron microscopy~~

C1602 Standard specification for mixing water used in the production of hydraulic cement concrete

C685 Standard Specification for Concrete Made by volumetric Batching and Continuous Mixing

C94 Standard Specification for Ready-Mixed Concrete

not going to download yet

For Slag: C441/C441M-17, C1073-18, C989/C989M-25

C348-21 Standard Test Method for Flexural Strength of Hydraulic-Cement Mortars

C917-~~25~~ 05 Standard Test Method for Evaluation of ~~Variability~~ Uniformity of Cement from a single source Based on Strength

C1709-22 Standard Guide for Evaluation of Alternative Supplementary Cementitious Materials for use in Concrete

C1697-25 Standard Specification for Blended Supplementary Cementitious Materials

C496-17 Standard Test Method for Splitting Tensile Strength of Cylindrical Concrete Specimens

C293-16 + C78-22 Standard Test Method for Flexural Strength of Concrete

C873-23 Standard Test Method for Compressive Strength of Concrete Cylinders Cast in place in Cylindrical molds

C1231-23 Standard Practice for Use of Unbonded Caps in Determination of Compressive Strength of Hardened Cylindrical Concrete Specimens

ACI Standards

~~ACI 318~~

ACI 214R

ACI 309 Guide for Concrete Consolidation

ACI 308.1-11 Specification for Curing Concrete