Predicting CO₂ Buoyant Flow Saturation in Heterogeneous Geologic Formations with Machine Learning

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Sub-meter scale barriers can determine migration pathways, speed of plume movement, and CO₂ storage capacity



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Increasing grain size contrast between matrix and laminae

(Increasing degree of heterogeneity)



S_{NWP}= 0.27%

S_{NWP}= 3.24%

S_{NWP}= 31.5%

S_{NWP}= 36.8%

CO₂ retained per grid block: 3% -> 48% CO₂ retained: 10% -> 21%

Why do modified invasion percolation simulations?

3D representation of the monitored CO₂ plume



Modified invasion percolation simulation result



Cavanagh & Haszeldine, 2014

Heterogeneity in natural geologic formations is affected by two major factors



Grain size

Trevisan et al., 2017

Rubin & Carter, 2005; Meckel et al., 2017

Bedform architecture

Data generation: modified invasion percolation simulations

- 59 bedform architectures X
- 40 grain size contrast cases X
- 50 stochastic realizations X
- = 118,000 simulations run





Rubin & Carter, 2005; Meckel et al., 2017; Trevisan et al., 2017

Data: first look



Model training: training and test set



Each bedform architecture model has all of its 40 grain size contrast cases included.



Model results: first model





Model building: with machine learning

- Add more features
 - Grain sorting
 - Geological entropy
 - Bedform descriptors
 - Planform shape
 - Shape and behavior through time
 - Crest orientation
 - Lamination type and shape

- Try different machine learning regression models
 - K nearest neighbors
 - Linear regression
 - Tree-based ensemble models
 - Random forest
 - Gradient-boosted trees
 - Artificial neural networks



Model building: feature selection

Matrix to laminae	ratio 1.00	-0.99	0.72	-0.46	0.01	0.23	0.26	0.27	0.00	-0.00	0.00	- 0.75
Global en	tropy -0.99	1.00	-0.74	0.46	0.04	0.24	0.25	0.24	0.00	0.00	0.00	
Entropic	scale 0.72	-0.74	1.00	-0.45	0.02	0.12	0.18	0.47	0.00	-0.00	0.00	- 0.50
Bottom filled vo	lume - 0.46	0.46	-0.45	1.00	0.15	0.29	0.08	0.25	0.00	-0.00	0.00	- 0.25
Lamination	type - 0.01	0.04	0.02	0.15	1.00	0.13	0.19	0.61	0.00	0.00	0.00	
Planform s	hape 0.23	0.24	0.12	0.29	0.13	1.00	0.46	0.67	0.00	0.00	0.00	- 0.00
Shape and behavior through	time 0.26	0.25	0.18	0.08	0.19	0.46	1.00	0.49	0.00	0.00	0.00	
Crest orient	ation 0.27	0.24	0.47	0.25	0.61	0.67	0.49	1.00	0.00	0.00	0.00	0.25
Grain so	orting 0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.76	0.00	0 50
Grain size co	ntrast -0.00	0.00	-0.00	-0.00	0.00	0.00	0.00	0.00	0.76	1.00	-0.38	0.50
Lamina median grai	n size 0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-0.38	1.00	0.75
	Matrix to laminae ratio -	Global entropy -	Entropic scale -	Bottom filled volume -	Lamination type -	Planform shape -	nd behavior through time -	Crest orientation -	Grain sorting -	Grain size contrast -	Lamina median grain size -	1.00

-1.00

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Model results: second model

 Random forest model





Model results: feature importance

Grain size contrast									
Lamina median grain size									
Bottom filled volume		Ī							
Lamination type_ripple									
Entropic scale									
Grain sorting_Extremely well sorted									
Global entropy									
Planform shape_3D-superimposed									
Grain sorting_Very well sorted									
Grain sorting_Moderately sorted									
Crest orientation_oblique									
Grain sorting_Well sorted									
Shape and behavior through time_variable									
Crest orientation_transverse									
Crest orientation_longitudinal									
Planform shape_2D									
0	.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	
BUREAU OF	Feature importance								

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Important features: grain sorting and laminae grain size



Important features: lamination type and shape

- High CO₂ saturation:
 - Continuous ripple lamination
- Low CO₂
 saturation:
 - Discontinuous cross-lamination

59

72

67

43a

Validation: experiments

Krishnamurthy, 2020

Important features: geological entropy and entrograms

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Bianchi & Pedretti, 2017; 2018

Economic

Geology

Potential model use case: upscaling critical CO₂ saturation for heterogeneous domains

