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Rational Development of Green Carriers for Viscosity Modifiers

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ABSTRACT

There is a growing effort to decrease the environmental impact of fracturing fluids by replacing the petroleum distillates with carriers that are more environmentally friendly. We created a robust approach for selecting candidate carriers leveraging experience from several fields.

We used a combination of experimental and computational methods to perform initial screening of candidate green solvents, then down-selected the best candidates for further testing.

At least one candidate solvent performed on par with the petroleum distillate control solvent.

The candidate solvents were able to control the rate at which hydroxypropyl guar increased viscosity in the aqueous solution.

This approach can simplify and expedite the process of developing new fracturing fluids with lesser environmental impact.

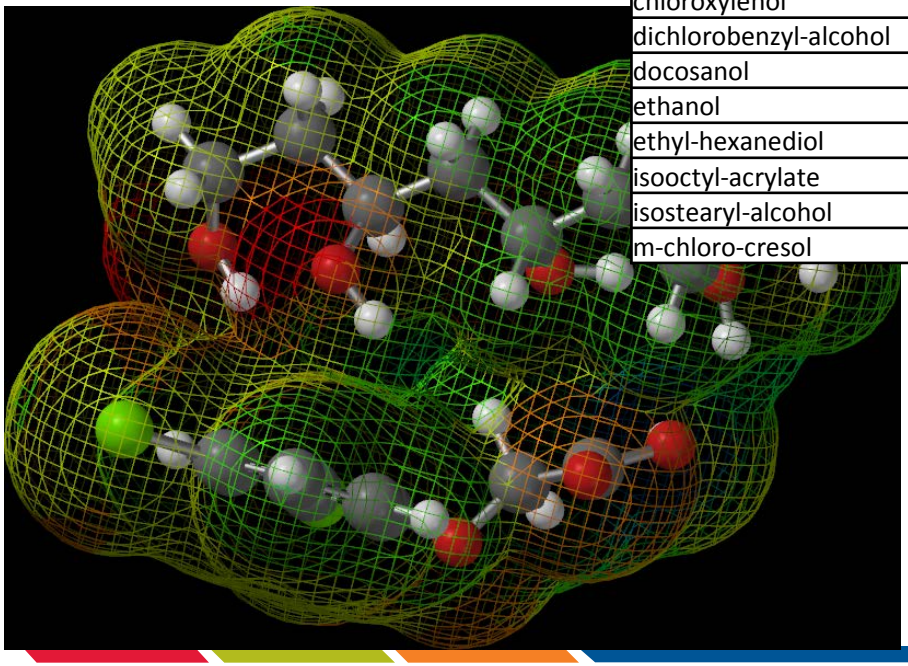
Approach to Chemical and Fluid Replacement

- Leverage formulation science, computational modeling and materials information tools to develop a systematic multi-dimensional framework for material replacements through functional performance attributes
- Incorporate existing tools used in adjacent fields
- Approach will speed development by
  - providing direction for experimentation
  - determining best candidates
  - eliminating poor candidates
  - providing insight into physical mechanisms

Tools from Adjacent Fields- BioPharma and AgFood Formulations

Some of the properties that must be examined when replacing a component in a formulation.

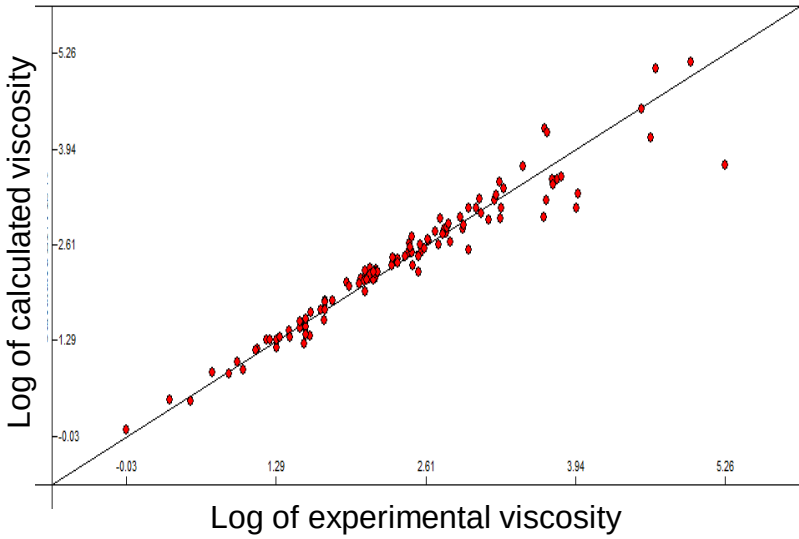
name	Molecular Formula	log Kow	Surface Tension (dyne/cm)	Density (g/cm3)	BP (C)	VP (mm Hg @ 25C)	Flash Point (F)	refractive index
water	water							1.329
IPA	IPA	0.16	22.6	0.791	73	81.33	53	1.376
octenidine	octen	10.78	35.8	0.94	610	0.001	612	
1,2,6-hexanetriol	C6H14O3	-1.75	48.8	1.113	323.1	0.001	330	1.483
benzyl-alcohol	C7H8O1	1.03	40.7	1.047	204.7	0.158	207.5	1.546
butyl-alcohol	C4H10O1	0.88	26	0.805	117.7	8.522	95	1.395
cetyl-alcohol	C16H34O1	7.25	31.1	0.835	310.9	0.001	275	1.448
chloro-butanol	C4H7O1Cl3	2.07	37.9	1.404	167	0.574	143.2	1.491
tetramethylene-clorohydrin	C4H9ClO	0.85	32.2	1.049	178.5	170.9	0.296	1.434
chloroxylenol	C8H9O1Cl1	3.35	40.2	1.183	246	0.018	222.6	1.558
dichlorobenzyl-alcohol	C7H6O1Cl2	2.24	46.7	1.392	268.4	0.004	239	1.582
docosanol	C22H46O1	10.44	31.7	0.839	375.9	0.001	288.6	1.454
ethanol	C2H6O1	-0.19	22.3	0.78	72.6	82.819	48	1.354
ethyl-hexanediol	C8H18O2	1.25	34.3	0.935	243	0.006	265	1.45
isooctyl-acrylate	C11H20O2	4.33	27.9	0.881	227.7	0.076	166.4	1.434
isostearyl-alcohol	C18H38O1	8.13	30.8	0.836	331.6	0.001	254.9	1.449
m-chloro-cresol	C7H7O1Cl1	2.5	42.1	1.228	230	0.045	172.6	1.565



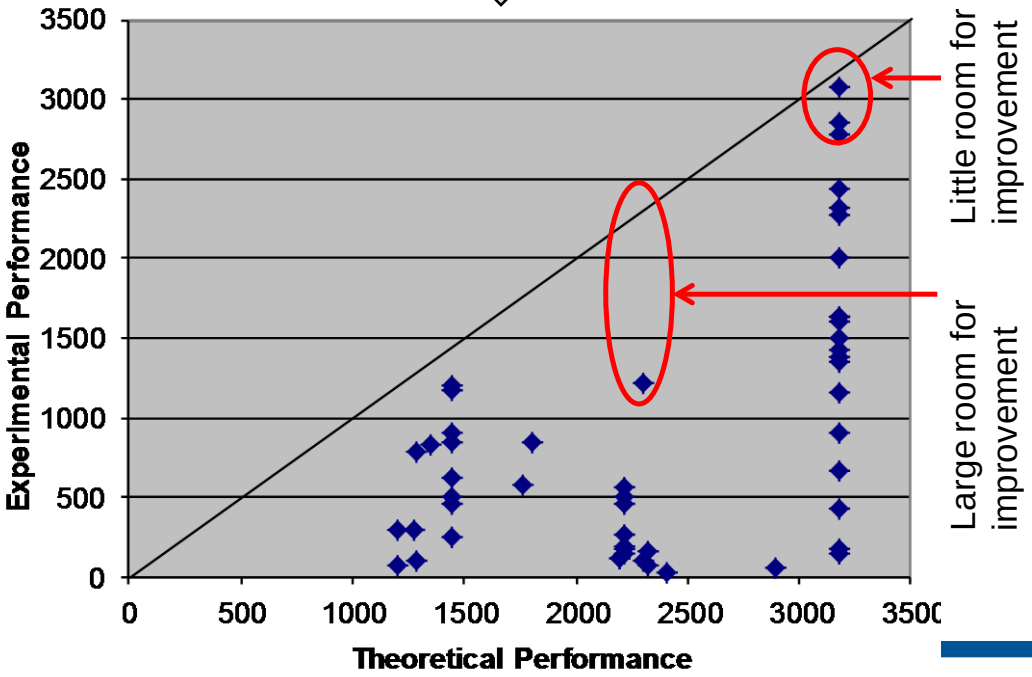
Interaction between a pesticide and its carrier polymer. These interactions control the release profile and are invaluable in formulation selection.

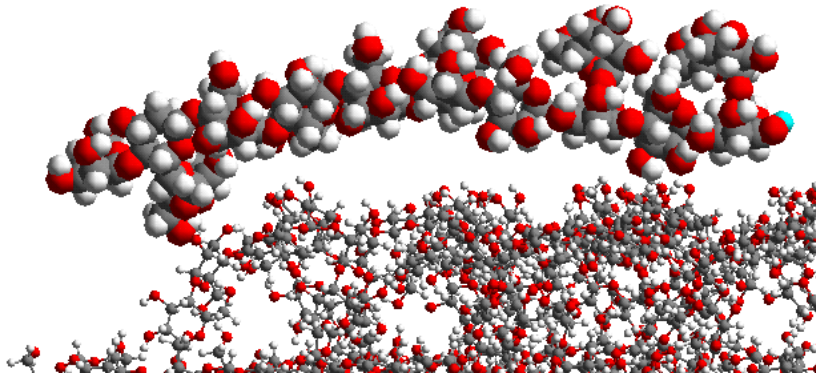
Tools from Adjacent Fields- Computational Chemistry and Materials

The accuracy possible when using computational tools to predict physical properties.



How use of knowledge tools can help in determining candidate materials for further development.





Atomistic models can provide details unavailable from experiments at the macroscopic scale.

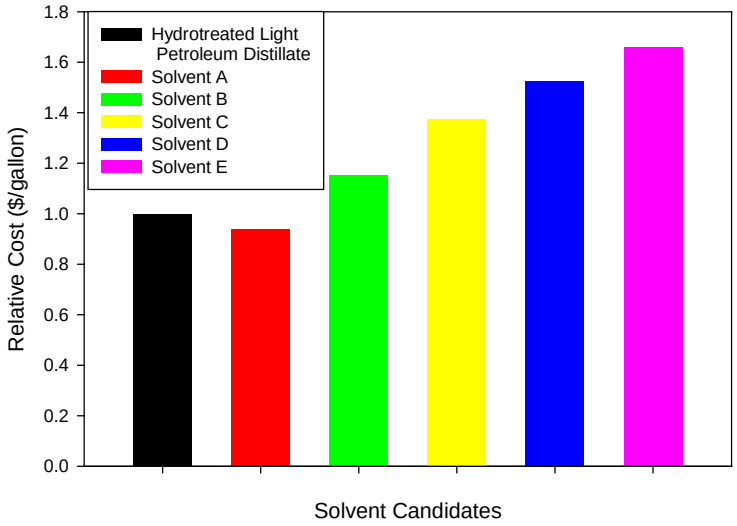
Case Study: Green Carriers for Viscosity Modifiers

- Define the problem
  - Determine relevant performance properties
  - Specify figure-of-merit and acceptable performance range
  - Understand interactions between *all* other formulation components
  - Derive mechanistic understanding of important phenomena
- Understand barriers to replacement
  - Must meet or exceed current performance
  - Must be lower cost than existing material
  - Must be compatible with existing field use conditions
  - Case for replacement strengthened if a new function is enabled
- “Green” does not sell anything on its own unless driven by regulations

Case Study: Green Carriers for Viscosity Modifiers

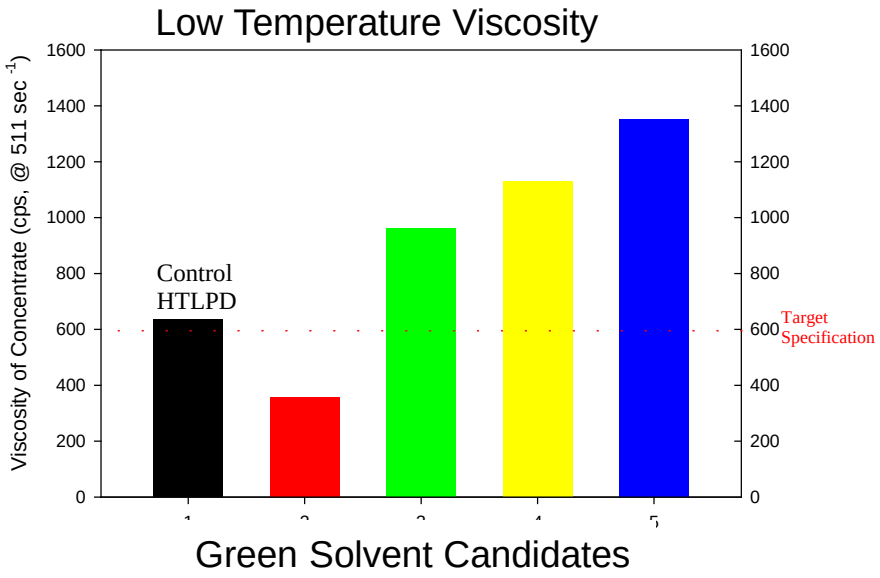
- Generate initial set of candidate molecules based on several criteria
  - Green Chemical Status: EPA Design for Environment (DfE); Toxicity, Biodegradability, VOC
- Use multiple parameters to perform initial down selection
  - Examine literature for known values of physical properties
  - Computational Chemistry approach to predict material interactions and phase behavior
  - Material cost and availability in bulk
  - Benchmark candidates vs control
  - Expected field performance based on SME understanding of mechanisms
- Conduct experiments focusing on best candidates

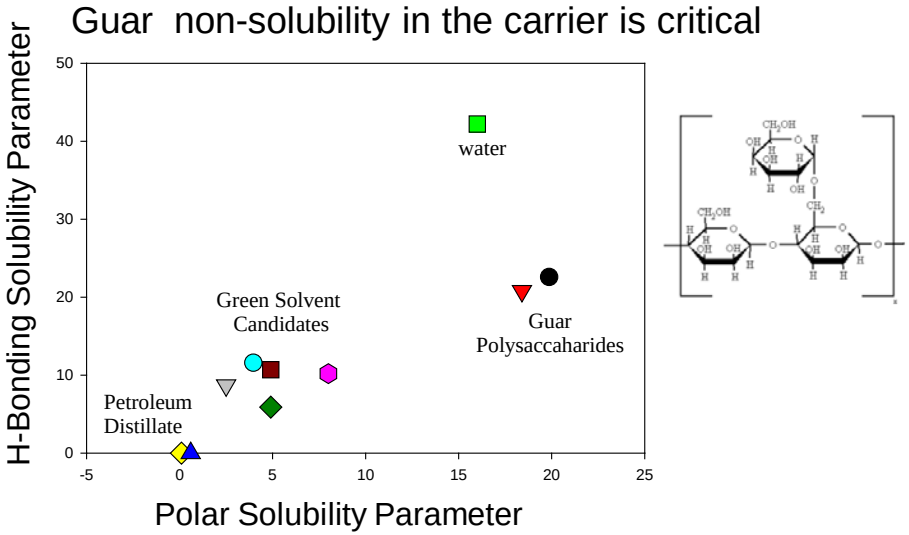
Cost and bulk availability are critical

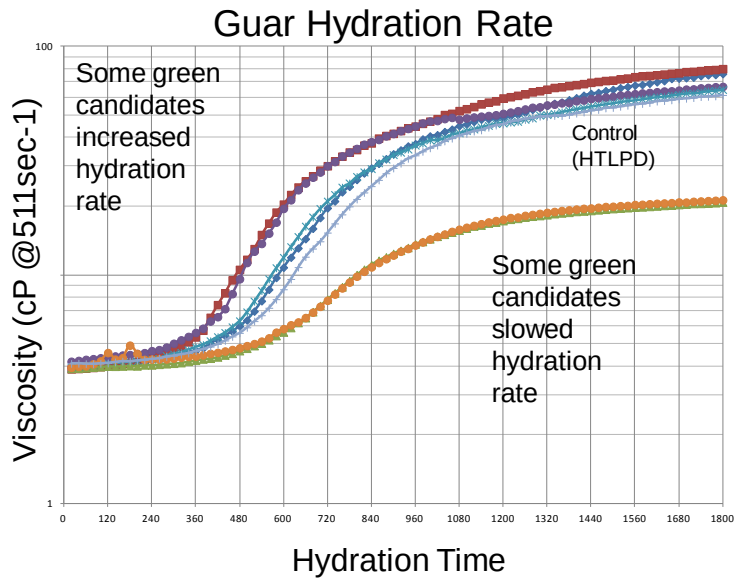


Case Study: Green Carriers for Viscosity Modifiers

- Evaluate control formulation vs candidate green replacements
  - Guar solubility
  - Viscosity
  - Hydration rate
- Demonstrate potential for additional functionality







Conclusions

- Have demonstrated a method for rational selection of replacement materials
- Method incorporates tools developed/utilized in adjacent and non-adjacent fields
- Case study on replacing the guar carrier in hydraulic fracturing fluids illustrated the primary steps
  - Define the requirements
  - Generate an initial set of candidate materials
  - Use known and predicted properties to down-select
  - Perform experimental testing on select set of candidates
  - Determine best choice(s) for field testing