Enhanced representation of thermal cracking chemistry in the context of bitumen partial upgrading

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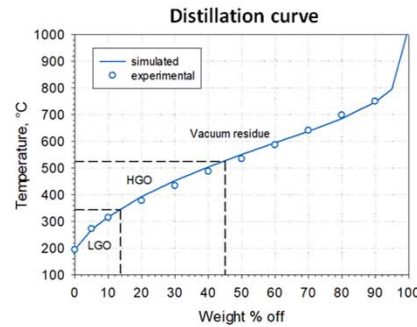Natural Resources Canada, CanmetENERGY Devon, AB, Canada T9G 1A8

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Bitumen composition modeling – bulk properties

Bitumen composition represented by an ensemble of 100k molecules
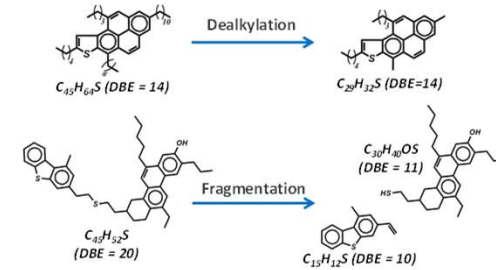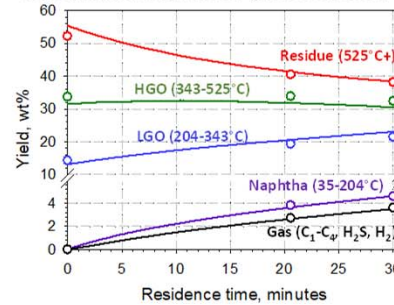

Bitumen feed properties

Property	Experimental	Simulated
Density at 15.6°C, g/mL	1.0146	1.0139
API gravity, °API	7.8	7.9
Carbon, wt%	83.38	83.94
Hydrogen, wt%	10.64	10.39
Sulfur, wt%	4.95	4.74
Nitrogen, wt%	0.49	0.41
Oxygen, wt%	0.54	0.52
SARA analysis		
Saturates, wt%	20.7	19.2
Aromatics, wt%	39.0	39.6
Resins, wt%	25.1	22.0
C_5 asphaltenes, wt%	19.3	19.3

Distillation curve

Visbreaker simulations – product yields

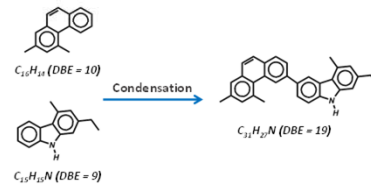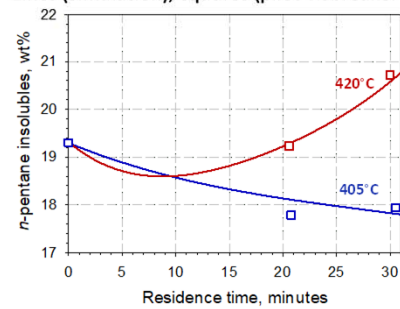Product yield structure evolves as a result of C-C and S-C bond cracking

Product yield profiles at 420°C -
Lines (simulation); circles (pilot visbreaker data)

Visbreaker simulations – asphaltenes

Condensation and dealkylation reactions drive formation of new asphaltenes

Asphaltene profiles at 405 and 420°C -
Lines (simulation); squares (pilot visbreaker data)

Visbreaker simulations – coke modeling

Coke is represented as a sub-fraction of pentane insolubles

Coke profiles at 390-430°C
Line (simulation); circles (pilot visbreaker data)