Non-ionic surfactants are used in hydraulic fracturing, which is an important technology for extracting oil and gas from impermeable rock. Data is fractionated with 10-20 barrels of water per barrel, which contains surfactants as lubricating agents and friction reducers. These compounds improve oil and gas recovery and carry water used to break the fractures in the strata, which allows oil and gas to be extracted. Half of the water returns to the surface, called backflow, and/or produced water, for deep well disposal.

The analysis of surfactants in produced and flowback water from hydraulic fracturing fluids using ion mobility mass spectrometry followed by quadrupole/time-of-flight mass spectrometry was utilized to analyze and “fingerprint” produced water samples and one flowback sample from different locations in the Denver-Julesburg (DJ) Basin in southeastern Colorado.

These groups of non-ionic surfactants polyethylene glycols (PEGs), polypolyethylene glycols (PPGs), and polyethylene glycol carboxylates (PEG-COOHs) were identified and developed that combined accurate masses with ion-mobility drift times for the identification of the three families of surfactants.

Isomers of PEGs, PPGs, and PEG-carboxylates are easily separated by UHPLC and identified by accurate mass with ion mobility MS using heatmaps.

Three different water samples (produced and flowback) from hydraulic fracturing are “fingerprinted uniquely” with ion mobility mass spectrometry. These studies equipped with a 1290 UHPLC system using the Agilent Model 6560 IMS were used from 10% A to 100% B in 30 min at a flow rate of 0.6 mL/min. Positive and negative ion electrospray with accurate mass measurement having a maximum drift time of 60 ms. Mobile phases A and B were water with 0.1% formic acid and acetonitrile, respectively. Sample volume was 20 µL. A linear gradient was used from 10% A to 100% B in 30 min at a flow-rate of 25 nL/min.

Experimental Conditions

The Agilent Model 6560 ion mobility mass spectrometer (Agilent Technologies, Inc., Santa Clara, CA) was used for these studies equipped with a 1290 UHPLC system using positive and negative ion electrospray with accurate mass measurement having a maximum drift time of 60 ms. Mobile phases A and B were water with 0.1% formic acid and acetonitrile, respectively. Sample volume was 20 µL. A linear gradient was used from 10% A to 100% B in 30 min at a flow-rate of 25 nL/min.

Results and Discussion

Results 3. Ion mobility mass spectrometry followed by quadrupole/time-of-flight mass spectrometry was utilized to analyze and “fingerprint” produced water samples and one flowback sample from different locations in the Denver-Julesburg (DJ) Basin in southeastern Colorado.

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3. Furthermore, the surfactants are then searched using the ion mobility test to find unknowns and identify them with accurate mass, MS-MS analysis, and the Kendrick mass defect.

Conclusions

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