Kerogen is an insoluble macromolecule, formed by degradation and condensation of different biomolecules. It is the source of all hydrocarbon generated from the organic rich shales. Despite its importance, it still remains to be one of the least studied components of shales. Previous work has indicated that shale with similar kerogen type and reservoir parameters such as thermal maturity, produces different amounts and type of hydrocarbons (HCs). This indicates that chemical structure and composition of kerogen play a major role in HC generation and production. To determine the sweet spots of HC extraction and increase the efficiency of HC production there is a need to better characterize chemical properties of kerogen at the molecular level.

We extracted kerogen from core samples collected from Mahantango and different zones of Marcellus Shale at the Marcellus Shale Energy and Environment Laboratory (MSEEL) site in Morgantown, West Virginia. Direct kerogen analytical techniques such as XPS (X-ray photoelectron spectroscopy), ATR-FTIR (Attenuated total reflection-Fourier transform infrared spectroscopy), 13C solid state NMR (Nuclear magnetic resonance) and Raman spectroscopy were used to determine the molecular structure of kerogen. Our results indicate that kerogen from all samples are mainly composed of highly aromatized carbon with minor amount of aliphatic carbon chains. The aromatic carbon fraction was dominated by aromatic bridgeheads carbon atoms and protonated aromatic carbon atoms indicating these carbon chains are refractory in nature and does not contribute significantly in hydrocarbon generation potential. Additionally, only minor amount of carbon chains such as mobile and immobile alkyl, methoxyl and alkyl-substituted aromatic carbons were observed, indicating that these functional groups are more prone to thermal degradation and have higher hydrocarbons generating potential.
Kerogen is an insoluble macromolecule, formed by degradation and condensation of different biomolecules. It is the source of all hydrocarbon generated from the organic rich shales. Despite its importance, it still remains to be one of the least studied component of shales. Previous work has indicated that shale with similar kerogen type and reservoir parameters such as thermal maturity, produces different amounts and type of hydrocarbons (HCs). This indicates that chemical structure and composition of kerogen play a major role in HC generation and production. To determine the sweet spots of HC extraction and increase the efficiency of HC production there is a need to better characterize chemical properties of kerogen at the molecular level.

We extracted kerogen from core samples collected from Mahantango and different zones of Marcellus shale at the Marcellus Shale Energy and Environment Laboratory (MSEEL) site in Morgantown, West Virginia. Direct kerogen analytical techniques such as XPS (X-ray photoelectron spectroscopy), ATR-FTIR (Attenuated total reflection-Fourier transform infrared spectroscopy), 13C solid state NMR (Nuclear magnetic resonance) and Raman spectroscopy were used to determine the molecular structure of kerogen. Our results indicate that kerogen from all samples are mainly composed of highly aromatized carbon with minor amount of aliphatic carbon chains. The aromatic carbon fraction was dominated by aromatic bridgeheads carbon atoms and protonated aromatic carbon atoms indicating these carbon chains are refractory in nature and does not contribute significantly in hydrocarbon generation potential. Additionally, only minor amount of carbon chains such as mobile and immobile alkyl, methoxyl and alkyl-substituted aromatic carbons were observed, indicating that these functional groups are more prone to thermal degradation and have higher hydrocarbons generating potential.

We extracted kerogen from core samples collected from Mahantango and different zones of Marcellus shale at the Marcellus Shale Energy and Environment Laboratory (MSEEL) site in Morgantown, West Virginia. Direct kerogen analytical techniques such as XPS (X-ray photoelectron spectroscopy), ATR-FTIR (Attenuated total reflection-Fourier transform infrared spectroscopy), 13C solid state NMR (Nuclear magnetic resonance) and Raman spectroscopy were used to determine the molecular structure of kerogen. Our results indicate that kerogen from all samples are mainly composed of highly aromatized carbon with minor amount of aliphatic carbon chains. The aromatic carbon fraction was dominated by aromatic bridgeheads carbon atoms and protonated aromatic carbon atoms indicating these carbon chains are refractory in nature and does not contribute significantly in hydrocarbon generation potential. Additionally, only minor amount of carbon chains such as mobile and immobile alkyl, methoxyl and alkyl-substituted aromatic carbons were observed, indicating that these functional groups are more prone to thermal degradation and have higher hydrocarbons generating potential.