Chapter 8

Recommendations for future work

The following recommendations are proposed for future work:

- Current nitrogen and sulfur functionality data is based on North American Carboniferous coal literature data. X-ray photoelectron spectroscopy (XPS) can be used to determine and quantify these organic heteroatom functionalities in South African coals. The heteroatoms play a role in solvent interaction behavior and therefore experimental values should lead to better model representation and behavior

- The type and distribution of oxygen functionalities constitutes the largest portion of the heteroatoms and play an important role in the formation of hydrogen bonds. Therefore, characterization of the organic oxygen functionality and distribution in the South African coals may lead to better model representations and solvent interaction simulations. X-ray photoelectron spectroscopy (XPS) and various chemical methods can be used to determine and quantify the organic oxygen in the South African coals. Fast neutron activation analysis (FNAA) could be conducted to obtain the precise oxygen concentration in these coals.

- A more advanced stop-motion videography method to study single-particle coal swelling can be designed. The use of a backlight may solve lighting issues observed in these experiments. Discoloration of the solvent during swelling resulted in particles being eliminated from the study (solvent to dark to conduct image analyses). A method should be investigated to reduce discoloration (for example, removal of solvent or the use of more solvent). Pre-extraction of the single-particles would solve the discoloration problem, but overshoot behavior will not be observed. The setup method should be designed in a manner that allows experiments to be conducted at various temperatures. Swelling data at various temperatures allows the calculation of the activation energies of swelling.

- A problem observed during X-ray computer tomography was the density difference between the solvent and coal. The density of the coal (ρ = 1.29 g/cm^3 for vitrinite-rich and ρ = 1.42 g/cm^3 for inertinite-rich coal) and the NMP solvent (ρ = 1.028 g/cm^3) were not sufficiently different to distinguish the solvent front in the coal particles during swelling. It is recommended that a higher density solvent be used (density considerable higher that that of the coal). The addition of an iodide group to the solvent could potentially solve this problem, but will change the coal-solvent swelling interaction. An alternative method that can be explored to study the solvent swelling is NMR imaging.

- A method to study the swelling of macerals on a microscopic level in real time should be investigated. This method will provide information on the individual maceral contribution to swelling and maceral synergism during solvent swelling. A possible concern with this method is that swelling will change the depth perception of field (as the particle swell it may move out of focus). Refocusing of the microscope during solvent swelling could lead to unreliable results. This type of setup needs to prevent solvent escaping to the atmosphere. Solvent escape during this method could lead to damage to the microscope equipment.

- It was observed that the mean random reflectance of vitrinite and inertinite (semifusinite and inertodetrinite) decrease with solvent swelling and extraction. The reasons for mean random reflectance changes are not understood and needs to be investigated. The change in reflectance could be attributed to chemical or physical changes. Structural changes would cause changes in reflectance and therefore solvent swelled and extracted residues needs to be structurally analyzed. High-resolution transmission electron microscopy, nuclear magnetic resonance spectroscopy and X-ray diffraction are possible methods that can be used.

- High-resolution transmission electron microscopy (HRTEM) micrograph interpretation needs to be examined thoroughly. HRTEM seems to be a promising tool to directly study the molecular structure of coal. Construction of molecular models directly from HRTEM micrographs (from 2D micrograph to 3D molecular structure) could lead to more representative molecular models.

- An automated method for model construction needs to be investigated. Model construction is a very time consuming process and suffers from personal bias. An automated method that can construct a model using analytical data could ensure fast and consistent models to be constructed.

- A coarse grain modeling method may allow the study of solvent swelling and extraction over longer simulation time frames. Various simulation algorithms and software packages should be evaluated for coal modeling.

- The proposed Permian-aged South African vitrinite-rich and inertinite-rich models can be used to investigate various other behaviors. Examples of behaviors that can be explored are: thermal expansion, pyrolysis, char formation, etc. The current models have only been tested for solvent interactions, and therefore testing for other behavior could lead to further verification of these models or the creation of better models.