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VAPOR PRESSURES AND HEATS OF VAPORIZATION OF PRIMARY COAL TARS

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"US/DOE Patent Clearance is not required prior to the publication of this document"

1.0 INTRODUCTION

1.1 MOTIVATION FOR THE STUDY

There is currently significant interest in the general area of coal pyrolysis, particularly with respect to development of comprehensive models of this complicated process. The interest derives from the central role of pyrolysis in all thermally-driven coal conversion processes-- gasification, combustion, liquefaction, mild gasification, or thermal beneficiation. There remain several key data needs, relative to proper modeling of any of these processes. Among these is a need for more reliable correlations for predicting the vapor pressures of the heavy, primary coal tars. Such information is clearly needed whenever the volatility or partitioning between phases, of the tarry products, is of major concern. For example, the mechanism of escape of coal tars is thought to involve evaporation of small degradation fragments into the vapor space around the particles or into bubbles within the particles.

The vapor pressure correlations that now exist for coal tars are quite crude. Sophisticated general correlative approaches are slowly being developed, based upon group contribution methods, or based upon some key functional features of the molecules. These are as yet difficult to apply to coal tars. The detailed group contribution methods, in which fairly precise structural information is needed, do not lend themselves well for application to very complex, poorly characterized coal tars. The methods based upon more global types of characterizations have not yet dealt much with the question of oxygenated functional groups. In short, only very limited correlations exist, and these are not considered reliable to even an order of magnitude when applied to tars.

The present project seeks to address this important gap in the near term by direct measurement of vapor pressures of coal tar fractions, by application of well-established techniques and modifications thereof. The principal objectives of the program are to: 1) obtain data on the vapor pressures and heats of vaporization of tars from a range of ranks of coal, 2) develop correlations based on a minimum set of conveniently measurable characteristics of the tars, 3) develop equipment that would allow performing such measurements in a reliable, straightforward fashion.

2.0 ACTIVITIES THIS QUARTER

The activities this quarter were limited because there was not yet a full-time graduate student working with the project. This problem has been resolved for the next quarter. Still, a number of steps were taken towards getting the project off to a start.

The equipment necessary for conducting the proposed measurements has been assembled in the lab of the PI, and been subjected to testing. For the effusion measurements, a TGA system is available. This method involves measuring the vapor pressure of an evaporating liquid sample indirectly, by measuring the rate of mass loss resulting from effusion of the vapor through a pinhole in a container containing the sample. Such effusion cells are commercially available, and a set has been ordered. The TGA is in working order.

The equipment needed for performing the flow saturation type measurements is also available. This consists basically of a gas chromatograph with flame ionization detectors. Initial attempts have been made to design small-volume, efficient saturators. These require some considerable further work.

3.0 PLANS FOR THE NEXT QUARTER

Initially, the graduate student will work on developing the already-established techniques for use in our laboratory. The goal is to push these techniques to measurement of vapor pressures of the highest molecular weight (lowest vapor pressure) materials, before resorting to the design of any new techniques to extend the range. This work will be performed with a series of well-defined pure compounds, because at this stage it is important to develop reliability of methods.

In addition to the vapor pressure measurements, it is at present anticipated that the measurements on the heats of vaporization of coal tars will be begun. There already exists a differential scanning calorimeter of suitable design for this purpose. It has a gas-purged sample compartment. We will work on low temperature tars, initially.

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