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DEW POINTS OF HOT GASES FROM COAL GASIFICATION PROCESSES

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### Objective and Scope

The long-range purpose of this research is to obtain fundamental physico-chemical data which, when coupled with theoretical results from molecular thermodynamics, will enable calculation of dew points in tar-containing gas mixtures at advanced temperatures and pressures.

### Summary of Progress to Date

Apparatus for measuring dew points has now been constructed. Preliminary efforts toward making the apparatus operational are now nearing completion.

Theoretical efforts for interpreting and correlating dew-point data are concentrated on statistical-mechanical and on kinetic theories. Relative advantages and disadvantages of both approaches are under consideration.

### Detailed Description of Technical Progress

This project consists of three sections, one theoretical and two experimental.

The theoretical section calls first, for a gas-phase equation of state appropriate to mixtures containing a variety of components. A suitable form for this equation of state has been identified and efforts toward its development are now underway. The equation is of the general van der Waals form, using the Carnahan-Starling equation for repulsive forces (1). Attractive forces are separated into nonpolar and polar contributions, each characterized by appropriate coefficients; these must be evaluated from experimental measurements. Using published experimental data for typical gases (e.g., hydrogen, methane, nitrogen, etc.), data reduction has been initiated to obtain the required coefficients from data reduction.

Second, the theoretical section calls for a group-contribution method to estimate vapor pressures of heavy hydrocarbons (and their derivatives) as a function of temperature. Two theoretical methods, one based on Prigogine's extended corresponding-states theory and the other based on the kinetic (coupled oscillator) theory of Berthoud, are under consideration (2,3). The relative advantages and disadvantages of the two methods have been scrutinized but it is not yet clear which of the two is more suitable for the purposes of this project.

The first experimental project concerns measurement of (small) vapor pressures of heavy hydrocarbons using Sinke's method. Five equilibrium cells have been constructed and a palladium-catalyzed combustion chamber has been completed. A constant-temperature bath is nearing completion. Calibration of the infra-red carbon dioxide detector is now underway. Some additional instruments for better temperature measurement have been ordered.

The second experimental project concerns measurement of solubilities of heavy hydrocarbons in compressed gases. Two equilibrium cells have been constructed and they are now being assembled with appropriate tubing and valves. A wet-test gas meter has been installed. Current focus is on the proper use of the analytical equipment, consisting of a gas-liquid chromatograph with an internal standard. The Beckman chromatograph appears to be working satisfactorily. Some heavy hydrocarbon chemicals have arrived and additional ones have been ordered. Heise gauges for pressure-measurement have been calibrated.

The rate of progress is consistent with that specified in the work plan.

Interest in our work was expressed by the Acurex Aerotherm Company (Mountain View, California). A research leader in that company inquired about our experiment methods since Acurex makes commercial instruments for coal processing plants, including instruments concerned with tar detection and analysis.

### Conclusions

At this early stage no technical conclusions can be expected. The project has been initiated as anticipated, progress is on schedule and no unusual or unexpected difficulties have been encountered.

### Literature Cited

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