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Interactions Between Trace Metals, Sodium and Sorbents in Combustion.

Quarterly Report No. 3

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INTRODUCTION

The proposed research is directed at an *understanding* of how to exploit interactions between sodium, toxic metals and sorbents, in order to optimize sorbents injection procedures, which can be used to capture and transform these metals into environmentally benign forms. The research will use a 17kW downflow, laboratory combustor, to yield data that can be interpreted in terms of fundamental kinetic mechanisms. Metals to be considered are lead, cadmium, and arsenic. Sorbents will be kaolinite, bauxite, and limestone. The role of sulfur will also be determined. The research is divided into five tasks.

Task 1: Combustor Modifications.

The existing laboratory combustor will be modified to allow injection of toxic metal surrogates, and withdrawal of particulate samples for subsequent analysis, without allowing leaks to impact the laboratory room environment.

Task 2: Screening Experiments.

Surrogate trace metals (3, listed above) will be injected through an otherwise "clean" gas flame stabilized in the combustor. Sorbents (3, listed above) will be injected through a port downstream. For each metal/sorbent pair, a statistically correct set of parametric experiments will be performed, quantitatively to determine the effects of a) sodium level, b) sulfur level, c) sorbent injection temperature, d) sorbent residence time, on trace metal capture. Measurements consist of the size segregated composition of the exhaust particulate matter. The objective function is the fraction of metal reactively captured by the sorbent. Solid and surface analyses will provide insight into mechanisms.

Task 3: Mechanisms.

Selected runs (6) from Task 2 will be repeated to obtain time resolved data on metal partitioning, with and without sodium and sulfur. The purpose will be to glean rates and mechanisms from size segregated particulate samples withdrawn. Advanced surface and solid analyses of sampled particulates will aid in mechanism building.

Task 4: Applications.

Three different, well characterized, pulverized coals will be burned, and the partitioning of the three toxic metals, in the presence of sorbents, examined, in the light of the mechanisms uncovered in Tasks 2 and 3. These mechanisms will also be used to determine the optimum application of sorbent injection in the presence of sodium and sulfur.

Task 5: Mathematical Modelling.

Tasks 2 through 4 will be accompanied by mathematical modeling. Empirical model building will be used in Task 2 to correlate, and interpolate the data. Deterministic and mechanistic modeling will be used to correlate and extrapolate the data of Tasks 3 and 4. This modelling will involve models of a) gas/solid reactions, and the appropriate particle size dependencies, b) gas phase reactions, either through partial/global equilibrium arguments (using CET89 software), or through CHEMKIN based detailed reactions, c) aerosol dynamics (using MAEROS), as required and appropriate.

PROGRESS FOR THIS QUARTER

Task 1: The design for the mini-baghouse and exhaust from the combustor is complete and is shown schematically on Figure 1 attached. The lower section of the furnace (A) will be replaced

by a 6" diameter stainless steel tube. Exhaust gas exits through a downward pointed exhaust (B). Large particles will be separated and collected in the ash trap (C). Flue gas is passed through a heated section of stainless steel pipe into the minibag house (D). Heating by heating tape is required in order to prevent condensation prior to, or inside, the bag house. A by-pass pipe (E) is available to protect the baghouse during start up, when all flue gas pipes are cold. From the baghouse the flue gas passes through a water jacketed condenser (to knock out the water of combustion), and then is sucked through a variable speed flue gas exhaust fan. The fan speed is so controlled as to maintain a negative pressure of at least 0.5" at the top of the furnace. Thus, toxic gases will be prevented from escaping into the laboratory.

Currently, all pieces of equipment, and supplies have been acquired. Stainless steel tubing was obtained from local (within 130 mile radius) scrap metal yards. The blower and varaible speed control, have also been purchased but not yet installed. We expect installation to be complete by December 1st, 1995.

Task 5: We have completed a methodology to allow the transfer of thermochemical data from the TAPP software into a form suitable for use by CET89. The TAPP thermochemical software directory has been installed in the Group's PC in its own subdirectory, TAPP,and has its own icon in the TAPP window. Windows should have over 15MB virtual memory available in order to run EXCEL v.5.0, TAPP, and FITDAT simultaneously.

TAPP to CET89 Procedure.

Start Windows. Click on TAPP icon. Select appropriate compound. Check thermochemical data, and make sure coefficients inluding C_4 are available. Remove all equation, coefficient and reference windows.

Export. Choose temperature increments such that there are no more than 30 (max allowed by FITDAT). Be sure that *entropy, specific heat, enthalpy* (H_T-H_{TREF}), $\Delta H_{formation}$ are the only items exported. Any additional items will mess up the format in the spreadsheet, and the remainder of the procedure will not work.

Save data. Change directory to c:\wolfgang\TAPP20 (previously in TAPP directory), and save with file name TAPPOUT.XLS.

ALT TAB switch to program manager and click on TAPP TO FITDAT Icon in TAPP window. This procedure opens Excel and requests an input file TAPPOUT.XLS. The message "External copy: The file is not valid", is OK. If excel cannot find its file it means that you have not changed directories as required.

Start methodology within Excel. USE ONLY CAPITALIZED LETTERS. At the conclusion of the procedure, the required files are found in c:\wolfgang\f32\fitdat as solid.dat etc. During the process the program goes into DOS, runs FITDAT, and returns. Do not be too fast in hitting the keyboard during this process. At the conclusion of the procedure the program asks whether you wish to complete a check of the thermodynamic data. It is recommended that this be done.

The spreadsheet produced allows comparison of the FITDAT produced thermochemical values with those originally produced by the file exported by TAPP. One can save this worksheet, which shows the comparison.

A future Quarterly Report will contain a coherent summary of the current status of our access to thermochemical data and reasonable equilibrium predictions.

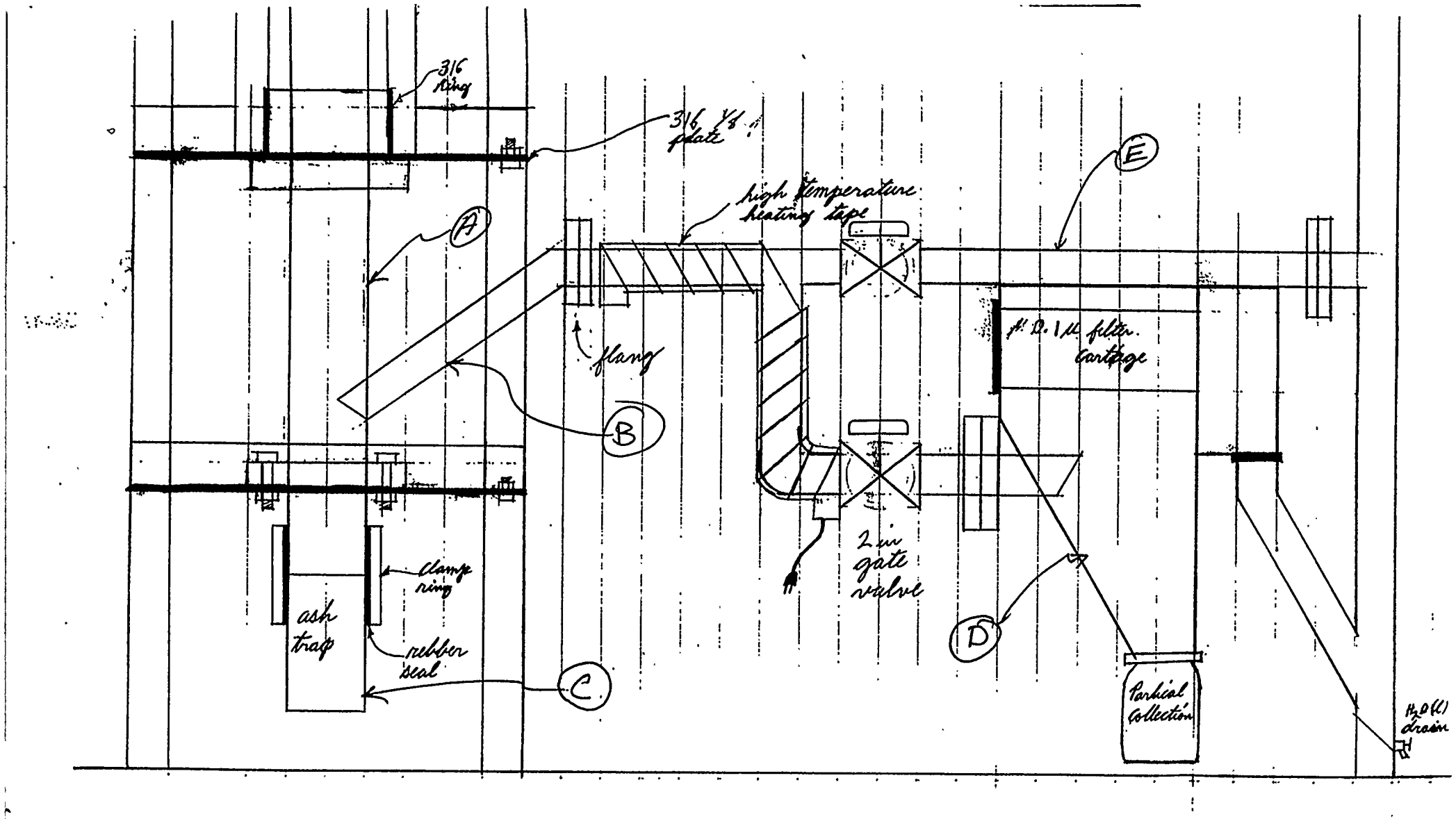


Figure 1: Furnace exhaust schematic

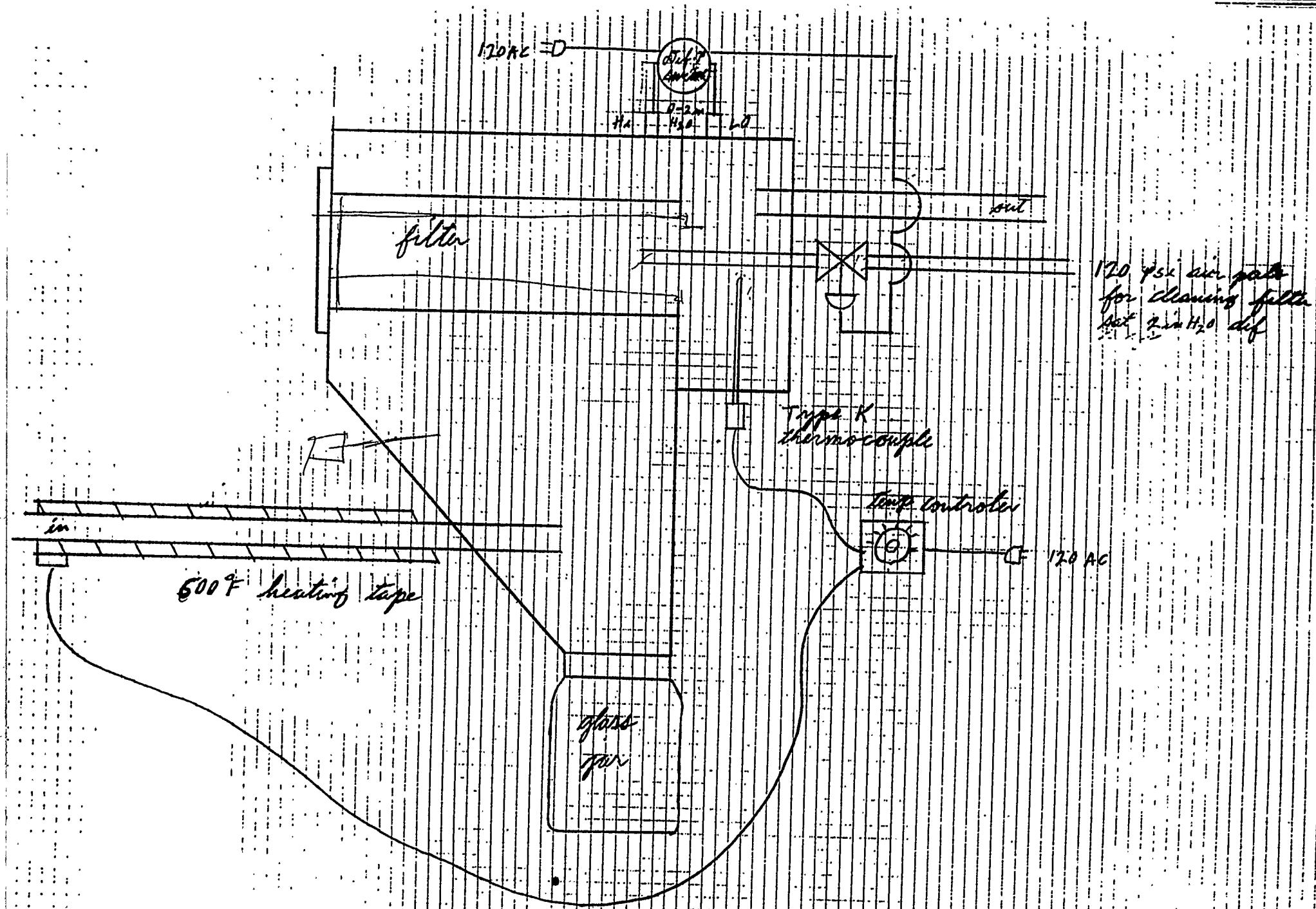
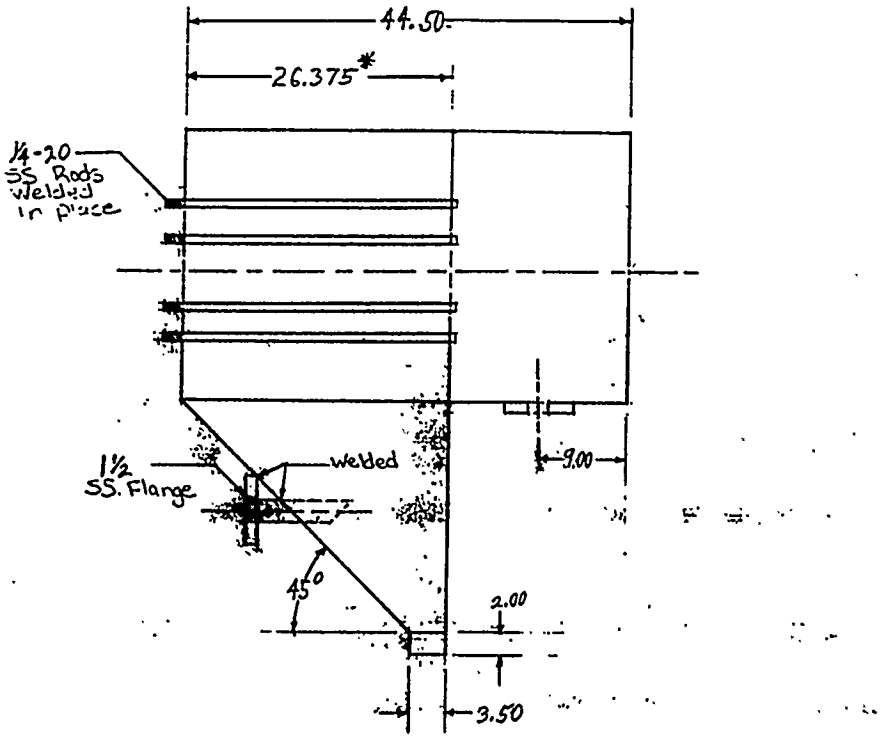
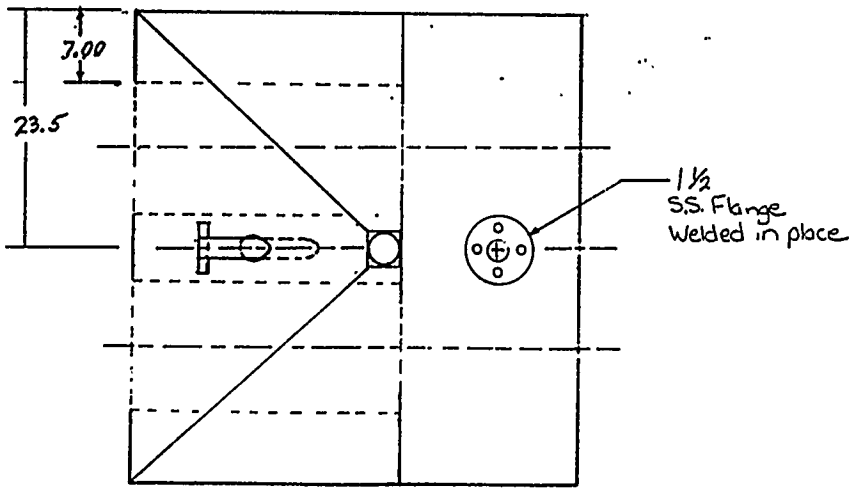
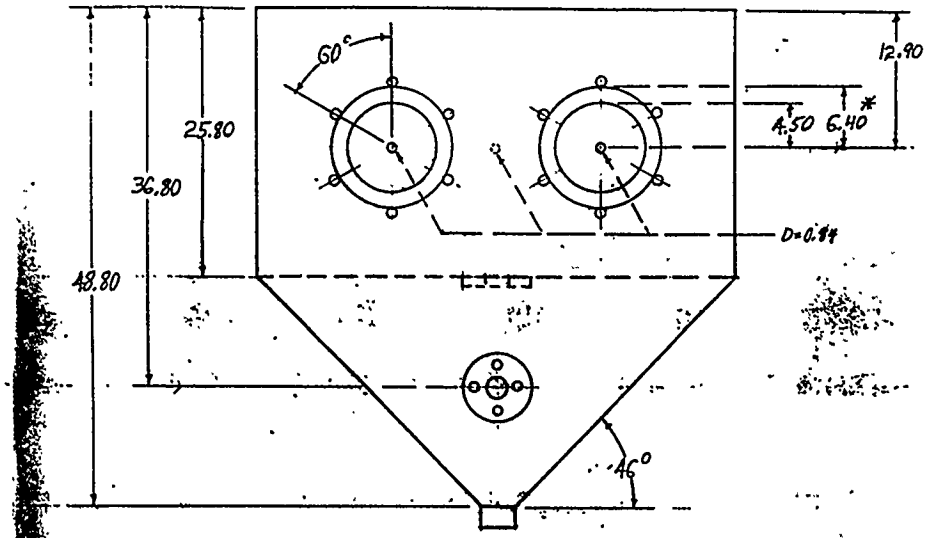


Figure 2 Mini Baghouse







* = Dimentions must be exact

Figure 3.: Mini Baghouse Details