# SECTION IV. TASK 4. APPLICATION OF INTEGRATED CODES Objective

The objectives of this task are to evaluate the integrated comprehensive codes for pulverized coal and fixed-bed reactors and to apply the codes to selected cases of interest to METC.

### Task Outline

This task will be accomplished in two subtasks, one for the entrained-bed lasting 57 months and one for the fixed-bed lasting 48 months. Each of these subtasks will consist of three components: 1) Simulation of demonstration cases on BYU computers; 2) Implementation on a work station at AFR; and 3) Simulations of demonstration cases on the workstation.

## IV.A. SUBTASK 4.A. - APPLICATION OF GENERALIZED, PULVERIZED-COAL CONPREHENSIVE CODE

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### <u>Objectives</u>

The objective; of this subtask are to 1) demonstrate application of the code by simulating reactors of interest to METC and 2) implement the code at METC and conduct training.

#### Accomplishments

A post-doctoral research associate was recruited and began work on this subtask. Potential application cases that were considered are shown in Table IV.A-1. Three of the cases (Coal Tech., ABB Combustion Engineering, and Airpol) are projects in the DOE Clean Coal Technology (CCT) program. Letter: were written to these three companies requesting available information or test data. Information has been received only from Coal Tech., and that case has been selected for application of the entrained-bed code under this subtask. A schematic diagram of the Coal Tech. combustor is shown in Fig. IV.A-1. Primary air and coal with sorbent are fed through numerous ports located in a ring on the west wall. Swirled secondary air is fed in an annulus outside of the primary stream. The flow is essentially two-dimensional. Because of the high swirl, the code will need to be modified to include the effect of centrifugal force on particle motion. The other application case will be the Texaco gasifier. Although the Texaco gasifier uses a slurry coal feed, it will be simulated with a dry coal feed.

#### <u>Plans</u>

Initiate simulation of Coal Tech. combustor and Texaco gasifier.

Name of Company	Type of Reactor	Location	Plant Capacity	Project Status
Texaco	entrained-flow gasifier	Barstow, CA	100 tons/day	in commercial operation
Shell Oil	entrained-flow gasifier	Royal Dutch Shell Research Lab	6 tons/day	project completed
Coal Tech. Corporation	cyclone combustor	Tampella Keeler Plant; Williamsport, PA	23 million Btu/hr	project completed
ABB Combustion Engineering	entrained-flow gasifier	Light & Power's Lakeside Stations Springfield, Sangamon County, IL	600 tons/day	under design and constructio
Airpol, Inc.	gas suspension absorption system	West Paducah, McCracken County, KY	10 MW	under design and constructio
Solar	coal-fired gas turbine combustor			
Allison	coal-fired gas turbine combustor			

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Table IV. A-1. Cases Considered for PCGC-2 Application

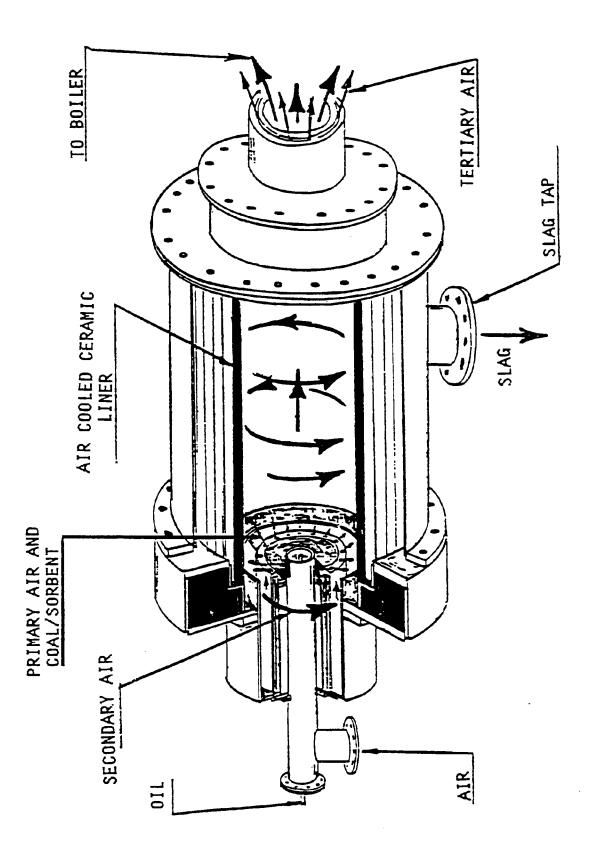


FIGURE IV. A-1. Coal Tech Corporation's air-cooled, cyclone coal combustor

### IY.B. SUBTASK 4.B. - APPLICATION OF FIXED-BED CODE

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### **Objectives**

The objective of this subtask is to apply the advanced fixed-bed code developed in Subtask 3.b. to simulate fixed-bed gasifiers of interest to METC.

### Accomplishments

The following application cases were approved by AFR and METC:

- 1. METC medium pressure, dry-ash gasifier.
- 2. BGC-Lurgi high pressure, dry-ash gasifier.
- 3. Wellman-Galusha atmospheric pressure, dry-ash gasifier.

Two new test cases of great potential interest were identified. Both are fixed-bed gasifiers integrated in gasification/combined cycle systems. One is a commercial, air-blown, dry-bottom, pressurized fixed-bed coal gasifier for the DOE/CCT project "Air-Blown/Integrated Gasification Combined Cycle Project." The other is an innovative, air-blown, dry-bottom, pressurized, fixed-bed coal gasifier for the DOE/METC project "Gasification Product Improvement Facility."

#### <u>Plans</u>

During the next quarter, work will continue to identify additional test cases for simulation, and the code will be applied to the cases of interest to METC.

#### REFERENCES

Annamalai K. and Ramalingham S.C., "Group Combustion of Char/Carbon Particles", Combustion and Flame, 70, 307 (1987).

Asay, B. W., "Effects of coal type and moisture content on burnout and nitrogenous pollutant formation," Ph.D. dissertation, Brigham Young University, Provo, UT, (1982).

Azuhata, S. H., P. O. Smoot, L. D. and Sowa, W. A., "Effects of flame type and pressure on entrained coal gasification," Fuel, 65, 1511-1515 (1986).

Ballal, G., Zygourakis, K., Ind. Eng. Chem. Res., 26, 1787, (1987).

Bhatia, S.K., Perlmutter, D.D., AIChE J., <u>26</u>, 379 (1980).

Bhatia, S.K., Perlmutter, D.D., AIChE, <u>27</u>, No. 2, 247 (1981).

Boardman, R. D., Smoot, L. D. and Brewster, B. S., Brigham Young University, "Subtask 2.G. - SOX/NOX Submodel Development," Chapter II.G. in Measurement and modeling of advanced coal conversion processes, 4th annual report, Solomon, P. R. et al., principal investigators, work performed under contract no. PE-AC21-85MC23075, U.S. Dept. of Energy/Morgantown Energy Tech. Center, Morgantown, WV, (1990).

Bohnen, C.F. and Huffman, D.R., <u>Absorption and Scattering of Light by Small</u> <u>Particles</u>, Wiley, New York (1983).

Borgwardt, R. H. and Bruce, K. R., "Effect of specific surface area on the reactivity of CaO with SO2," AIChE J., 32, 239-246 (1986).

Borgwardt, R. H., Bruce, K. R. and Blake J., "An investigation of product-layer diffusivity for CaO sulfation," IEC Res., 26, 1993-1998 (1987).

Brewster, B. S., Smoot, L. D. and Berrondo, S. K., Brigham Young University, "Subtask 3.A. - Integration of advanced submodels into entrained-flow code, with evaluation and documentation," Chapter III.A. in Measurement and modeling of advanced coal conversion processes, 4th annual report, Solomon, P. R. et al., principal investigators, work performed under contract no. DE-AC21-86MC23075, U.S. Dept. of Energy/Morgantown Energy Tech. Center, Morgantown, WV, (1990).

Brown, B.W., "Effect of coal type on entrained flow gasification," Ph.D. Dissertation, Brigham Young University, Provo, UT, (1984).

Calo, J.M., Perkins, M.T., Carbon, <u>25</u>, 395, (1987).

Cannon, J. N., Queiroz, M. and Webb, B. W., "Full-scale testing of an 80 MWe tangential coal fired power plant," 14th Annual Energy Sources Technology Conference and Exhibition, R. Ruiz, ASME, PD vol. 33, Houston, TX, January 20-23, 49-56 (1991).

Costa, M., Costen, P., Lockwood, F. C. and Mahmud, T., "Detailed measurements in and modelling of an industry-type pulverised-coal flame," Twenty-Third Symposium (International) on Combustion, The Combustion Institute, Pittsburgh, PA, 973-980 (1990).

Davini, P., DeMichele, G. and Bertacchi, S., "Reaction between calcium-based sorbents and sulfur dioxide - A thermogravimetric investigation," Fuel, 70, 201-204 (1991).

DeSoete, G. G., Overall reaction rates of NO and  $N_2$  formation from fuel nitrogen, 15th Symposium (International) on Combustion, The Combustion Institute, Pittsburgh, PA, 1093-1102 (1975).

Du, Z., Sarofim, A.F., Longwell, J.P., Energy & Fuel, <u>4</u>, 296, (1990).

Dutta, S., Wen, C.Y., Ind. Eng. Chem. Process Design Develop. 16, 31, (1977).

Eatough, C., "Controlled profile reactor design and combustion measurements," Ph.D. dissertation, Brigham Young University, Provo, UT, (1991).

Faires, L. M., Apel, C. T., Niemczyk, T. M. Applied Spectroscopy Vol. 37, No. 6, pp 558-563, 1983.

Floess, J.K., Longwell, J.P., Sarofim, A.F., Energy & Fuel, 2, 18, (1988).

Gan, H., Nandi, S.P., and Walker, P.L., Jr., Fuel, 51, 272, (1972).

Gavalas, G.R., AIChE J., <u>26</u>, 577, (1980).

Goetz, G. J., Nsakala, N. Y., Patel, K. L. and Lao, T. C., "Combustion and gasification kinetics of chars from four commercially significant coals of varying rank," Second Annual Conference on Coal Gasification, EPRI, Palo Alto, CA, October, (1982).

Gopalakrishnan, R. and Seehra, M. S., "Kinetics of the high temperature reaction of  $SO_2$  with CaO particles using gas-phase fourier transform infrared spectroscopy," Energy & Fuels, 4, 226-230 (1990).

Gullett, B. K. and Bruce, S. R., "Pore distribution changes of calcium-based sorbents reacting with sulfur dioxide," AIChE J., 33, 1719-1987 (1987).

Gutierrez, M.C., Cukierman, A.L., Lemcoff, N.O., Fuel, <u>66</u>, 722, (1987).

Habib, Z.G. and Vervisch, P. Comb. Sci. & Technol., 59, 261, (1988).

Haji-Sulaiman, M. Z. and Scaroni, A. W., "The calcination and sulphation behavior of sorbents in fluidized bed combustion," Fuel, 70, 169-176 (1991).

Hashimoto, K., Silveston, P.L., AIChE J., 19, 259, (1973).

Hobbs, M. L., Radulovic, P. T., and Smoot, L. D., "Prediction of Effluent compositions for Fixed-Bed Coal Gasifiers," submitted to <u>Fuel</u>, (1991a).

Hobbs, M. L., Radulovic, P. T., and Smoot, L. D., "Modeling Fixed-Bed Coal Gasifiers," submitted to <u>AIChE\_Journal</u>, (1991b).

Hottel, H.C. and Sarofim, A.F. "Radiative Transfer", McGraw Hill, NY, (1967).

Jamaluddin, A. S. and Smith, P. J., Prediction of radiative heat transfer in cylindrical furnaces, Western States and Canadian Sections, The Combustion

Institute, Banff, Canada, April, (1986).

Jost, M., Leslie, I. and Kruger, C. H., "Pulverized Coal Combustion. Final Report, December 17, 1981-June 17, 1983," DOE/PC/30177-4, Stanford Univ., Palo Alto, CA, (1983).

Ko, G. H., Sanchez, D. M., Peters, W.A., and Howard, J. B., "Correlations for Effects of Coal Type and Pressure on Tar Yields from Rapid Devolatilization," <u>Twenty-Second Symposium (International) on Combustion</u>, The Combustion Institute, Pittsburgh, Pennsylvania, 115 (1988).

Kocaefe, D., Karman, D. and Steward, F. R., "Interpretation of the sulfation rate of CaO, MgO, and ZnO with SO<sub>2</sub> and SO<sub>3</sub>," AIChE J., 23, 1835-1843 (1987).

Levy, J. M., Chen, L. K., Sarofim, A. F. and Béer, J. M., NO/char reactions at pulverized coal flame conditions, 18th Symposium (International) on Combustion, The Combustion Institute, Pittsburgh, PA, 111-120 (1981).

Lizzio, A.A., Piotrowski, A., Radovic, L.R., Fuel, <u>67</u>, 1691, (1988).

Lockwood, F. C. and Mahmud, T., "The prediction of swirl burner pulverised coal flames," Twenty-Second Symposium (International) on Combustion, The Combustion Institute, Pittsburgh, PA, Seattle, WA, August 14-19, 165-173 (1988).

Lockwood, F. C., Salooja, A. P. and Syed, S. A., "A prediction method for coal-fired furnaces," Comb. Flame, 38, 1-15 (1980).

Lockwood, F. C., Rizvi, S. M. A., Lee, G. K. and Whaley, H., "Coal combustion model validation using cylindrical furnace data," Twentieth Symposium (International) on Combustion, The Combustion Institute, Pittsburgh, PA, 513-522 (1984).

Lockwood, F. C. and Salooja, A. P., "The prediction of some pulverized bituminous coal flames in a furnace," Comb. Flame, 54, 23-32 (1983).

Mahajan, O.P., Yarzab, R., Walker, Jr., P.E., Fuel, <u>57</u>, 643, (1978).

Markham, J. R. and Serio, M. A., Brigham Young University, "Subtask 2.C. -Secondary reaction of pyrolysis products and char burnout submodel development and evaluation," Chapter II.C. in Measurement and modeling of advanced coal conversion processes, 4th annual report, Solomon, P. R. et al., principal investigators, work performed under contract no. DE-AC21-86MC23075, U.S. Dept. of Energy/Morgantown Energy Tech. Center, Morgantown, WV, (1990).

Menguc, M.P. and Viskanta, R., "A Sensitivity Analysis for Radiative Heat Transfer in a Pulverized Coal-Fired Furnace," <u>Combustion Science and Technology</u>, 51, p. 51 (1987).

Milne, C. R., Silcox, G. D., Pershing, D. W. and Kirchgessner, D. A., "Calcination and sintering models for application to high-temperature, short-time sulfation of calcium-based sorbents," Industrial & Engineering Chemistry Research, 29, 139-149 (1990).

Mitchell, R. E., "The influence of the mineral matter content of coal on the temperatures and burning rates of char particles during pulverized coal combustion," Sixth Annual International Pittsburgh Coal Conference Proceedings,

Pittsburgh, PA, September 25-29, 32-52 (1989).

Mitchell, R.E., "The Influence of the Mineral Matter Content of Coal on the Temperatures and Burning Rates of Char Particles During Pulverized Coal Combustion," The Sixth Annual International Pittsburgh Coal Conference, Pittsburgh, Pennsylvania, Vol. 1, 32 (1989).

Miura, K., Silveston, P.L., Energy & Fuels, <u>3</u>, 243, (1989).

Newton, G. H., Harrison, D. J., Silcox, G. D. and Pershing, D. W., "Control of SOx emissions by in-furnace sorbent injection: Carbonates vs. hydrates," Environ. Prog., 5, 140-144 (1986).

Pace, R.S., "Titanium as a Tracer for Determining Coal Burnout," M.S. Thesis, Brigham Young University, Dept. of Chem. Eng., (1982).

Parkinson, A.R., Balling, R.J., and Free, J.C., "OPTDES.BYU: A Software System for Optimal Engineering Design," Proceedings ASME Int. Computers in Eng. Conf., Las Vegas, NV (1984).

Radovic, L.R., Walker, P.L., Jenkins, R.G., Fuel, <u>62</u>, 849, (1983).

Silcox, G. D., "Analysis of the SO2-lime reaction system: Mathematical modeling and experimental studies emphasis on stoker applications," Ph.D. dissertation, The University of Utah, (1985).

Smoot, L. D. and Smith, P. J., Coal combustion and gasification, Plenum, New York (1985).

Soelberg, N.R., "Local measurements in an entrained coal gaisifer," MS Thesis, Brigham Young Unviersity, Provo, UT, (1983).

Solomon, P. R., Serio, M. A., Carangelo, R. M. and Markham, J. R., "Very rapid coal pyrolysis," Fuel, 65, 182-194 (1986).

Solomon, P.R.; Serio, M.A.; Hamblen, D.G.; Smoot, L.D. and Brewster, B.S., "Measurement and modeling of advanced coal conversion processes," AFR Fourth Annual Report, (1990).

Su, J.L., Perlmutter, D.D., AIChE J., <u>31</u>, No. 6, 973 (1985).

Thimsen, D., Maurer, R. E., Poole, A. R., Pui, D. Y. H., Liu, B. Y. H., and Kittelson, D. B., "Fixed-Bed Gasification Research using U.S. Coals," 1-19, U.S. Bureau of Mines Contract H0222001, Final Report, (1984-1985).

Tichenor, D.A., Mitchell, K.R., Hencken, K.R., Niksa, S., "Simultaneous In Situ Measurement of the Size, Temperature and Velocity of Particles in a Combustion Environment," <u>Twentieth Symposium (International) on Combustion, The Combustion Institute</u>, Pittsburgh, PA, p. 1213 (1984).

Tseng, H.P., Edgar, T.F., Fuel, <u>64</u>, 373, (1985).

Tseng, H.P., Edgar, T.F., Fuel, <u>63</u>, 385, (1984).

.

van Krevelen, D.W., Properties of Polymers, Elsevier, NY, (1976).

Varma, S. A. and Pratt, D. T., Anisotropic and multiple scattering of thermal radiation in pulverized coal combustors, 17th Symposium (International) on Combustion, Pittsburgh, PA, (1978).

Varma, S. A., "Radiative heat transfer in a pulverized-coal flame," Chapter 5 in Pulverized coal combustion and gasification, Eds., Plenum Press, New York, NY, 83-106 (1979).

Young, B.C. and Smith, I.W., "The Kinetics of Combustion of Petroleum Coke Particles at 1000 to 1800 K: The Reaction Order," Eignteenth Symposium on Combustion/The Combustion Institute, 1249 (1981).

Waters, P.L., Fuel, 41, 3, (1962).

Westenberg, A. A., "Kinetics of NO and CO in lean, premixed hydrocarbons air flows," Comb. Sci. Tech., 9, 59 (1971).

Zygourakis, K., "Pyrolysis and Gasification of Coal Particles at High Temperatures" Contract Report DE-FG22-87PC79930, (1989).