Functional-Group, Depolymerization, Vaporization, Cross-linking Model

What is FG-DVC

The Functional-Group, Depolymerization, Vaporization, Cross-linking (FG-DVC) model is a comprehensive code for predicting yields and compositions of coal-pyrolysis products (gas, tar, and char). The quantification of gas-phase NOx precursors is also possible. The code is particularly useful in modeling high heating rate processes, where experimental data are difficult to collect. Coal switching, blending, and co-firing of biomass and coal are other applications. The model is based on the fundamentals of coal chemistry and physics. The model has recently been extended to biomass and to processes involving large coal particles. For coals, the minimum input is ultimate analysis, but more reliable results are obtained if input files are generated on the basis of TG-FTIR analysis available from Advanced Fuel Research. (TG-FTIR = thermogravimetric analyzer combined with Fourier transform infrared analysis of evolving products.) In the case of biomass, we recommend input files based on TG-FTIR data. The model is available as a stand-alone version and as a submodel for computational fluid dynamics (CFD) codes.

Features

Diverse feedstocks:

- coal
- biomass
- waste materials (e.g., waste tires)

The following information provided as a function of extent of devolatilization (e.g., pyrolysis time):

- Gas, tar, and char yields
- Elemental composition of gas, tar, and char
- Molecular weight distribution of tar
- Information on coal softening and fluidity
- Detailed speciation and quantification of volatile products:

- Tar
- H_2O
- CO_2
- CO
- CH_4
- C_2H_4
- NH_3
- HCN
- COS
- SO_2

For biomass, additionally:

- formaldehyde
- acetaldehyde
- formic acid
- acetic acid
- methanol
- phenol
- acetone
- levoglucosan

- The effect of pressure taken into account
- Capability for integration with Computational Fluid Dynamics (CFD) codes

- FLUENT
- PCGC-2 (pulverized coal combustion/gasification - Brigham Young University)
- AIOLOS (University of Stuttgart)
- MBED-1 (fixed beds - Brigham Young University)
- FBED-1 (fixed beds - Brigham Young University)
- MFIX (fluidized beds – U.S. Department of Energy)

- Stand-alone versions available on multiple platforms

- PC (DOS, Windows 95 / 98 / NT)
- UNIX
- Macintosh (under development)

- Extensive customer support available from the model developer, Advanced Fuel Research, Inc. (includes TG-FTIR characterization of unusual
- Model Input

- Elemental composition of coal or biomass
- Pyrolysis temperature as a function of time
- In the case of biomass, some coals, and non-standard feedstocks, TG-FTIR analysis (a thermogravimetric analyzer combined with Fourier transform infrared analysis of evolving products) – available from Advanced Fuel Research, Inc.

Applications

- Coal-conversion processes: pyrolysis, gasification, combustion, liquefaction
- Coal switching
- Coal blending
- Co-firing of biomass and coal
- Biomass conversion: pyrolysis, gasification, and combustion

Modeling Approach

The modeling approach used in FG-DVC is phenomenological in nature. A suite of well-characterized coals was selected to form an FG-DVC database (library coals), and pyrolysis behavior of these coals was extensively studied using TG-FTIR analysis, pyrolysis Field Ionization Mass Spectrometry (FIMS), Gieseler fluidity, solvent swelling and solvent extraction. Based on this information, three FG-DVC input files were created for each library coal: (1) kinetic file; (2) composition file; and (3) polymer file. The first two files describe the kinetics of gas-product evolution and the amounts of precursor material for each volatile species. A set of independent, first-order reactions with Gaussian activation-energy distributions is used for the kinetic model. The polymer input file contains information on the coal's swelling and fluid behavior. The library coals can be represented as a network of grid nodes in the so-called van Krevelen diagram (a plot of H/C versus O/C atomic ratios). The required three FG-DVC input files can be generated for any coal, as illustrated in Figure 1. Elemental composition data for an untested coal are plotted in the van Krevelen diagram, and input parameters are interpolated from among input parameters of the three nearest library coals (triangular interpolation). In this way, elemental composition is the only input information that is needed to run the FG-DVC code. For unusual feedstocks, custom input files can be created at AFR.

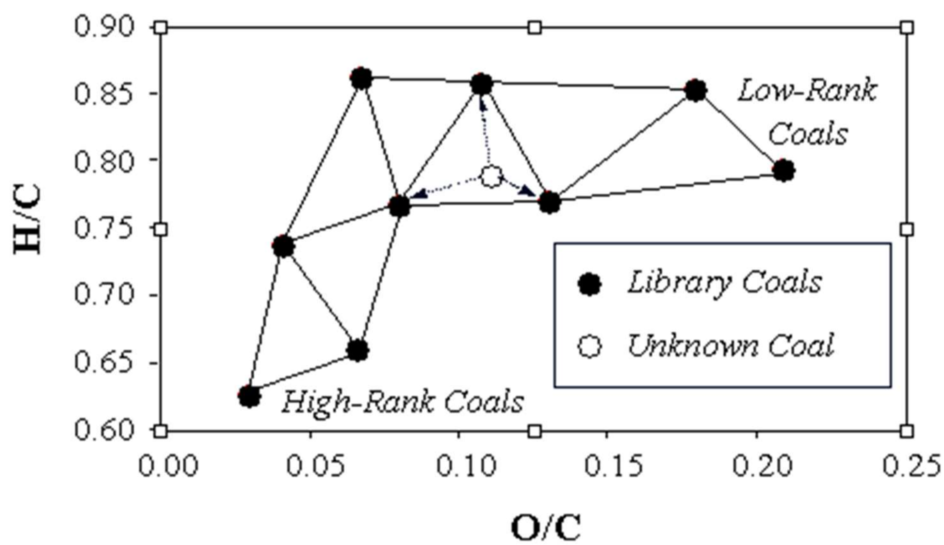

Figure 1. Illustration of an interpolation scheme used to create FG-DVC input files for a coal with an unknown pyrolysis behavior.

Model Validation

The FG-DVC model has been extensively validated against experimental data, and more detailed information on model validation can be found in The FG-DVC Model Description and Validation fact sheet. For the sake of illustration, results of blind model-prediction tests are shown in Figure 2. An independent testing program was carried out on behalf of Electric Power Research Institute (EPRI), and the tests involved drop-tube pyrolysis experiments performed at PowerGen. A set of eight international coals was used, and AFR was provided only with their proximate and ultimate analyses in addition to the nominal pyrolysis conditions (a linear temperature ramp at 2 x 104 K/s from room temperature to 1613 K, followed by an isothermal treatment at 1613 K for 150 milliseconds). The dotted lines in Figure 2 indicate the approximate range of uncertainty in experimental data, and solid symbols represent the FG-DVC model predictions. It can be seen that the agreement is good.

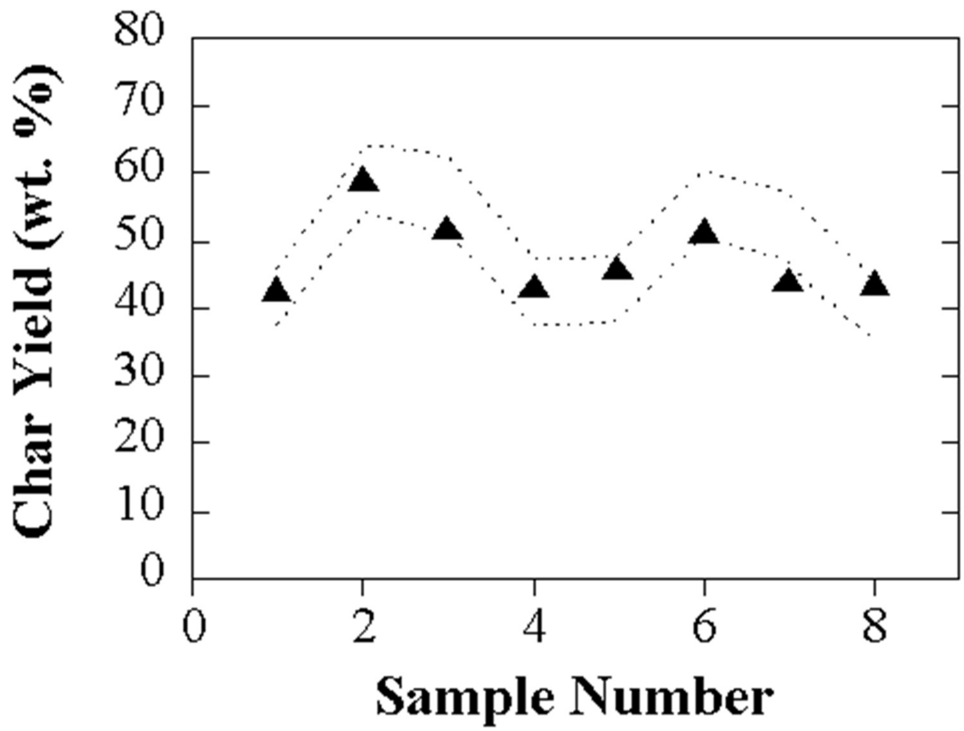

Figure 2. Comparison of PowerGen drop-tube pyrolysis data with FG-DVC model predictions. Dotted lines indicate the uncertainty limits of experimental data, and solid symbols represent model predictions.

Further Information

The following FG-DVC fact sheets are available:

- The FG-DVC Model Description and Validation
- A List of Publications on the FG-DVC Model
- FG-DVC Ordering Information

Inquiries about the FG-DVC model should be directed to Dr. Marek A. Wójtowicz, Vice-President, Clean Energy and Carbon Materials, Advanced Fuel Research, Inc., East Hartford, CT 06108, USA; tel. +1 (860)528-9806, fax +1 (860)528-0648, e-mail: marek@AFRinc.com.

Users of the FG-DVC Model

A partial list of laboratories which have used the FG-DVC Model.

U.S.A.

Name	**Location**
ABB - Power Plant Laboratories	Windsor, CT
Riley Stoker Corporation	Worcester, MA
Babcock and Wilcox Co.	Alliance, OH
Foster Wheeler Development Corp.	Livingston, NJ
Factory Mutual Research Corp	Norwood, MA
BOC Group Technical Center	Murray Hill, NJ
CRS Sirrine Engineers, Inc.	Greenville, SC
Bechtel Corp	San Francisco, CA
Department of Energy, NETL	Morgantown, WV
Department of Energy, NETL	Pittsburgh, PA
National Institute of Standards and Technology	Gaithersburg, MD
National Renewable Energy Laboratory	Golden, CO
FAA Technical Center	Atlantic City, NJ
Brown University	Providence, RI
Brigham Young University	Provo, UT
Virginia Polytechnic Institute	Blacksburg, VA
Oregon State University	Corvallis, OR
University of Utah	Salt Lake City, UT

Overseas

Name	**Location**
Institut Français du Pétrole	Rueil - Malmaison, France
AEA Technology	Oxfordshire, UK
DMT Gesellschaft	Essen, Germany
Insituto de Carboquimica	Zaragoza, Spain
Instituto Nacionel Del Carbon	Oviedo, Spain
Reatech	Roskilde, Denmark
Swedish National Testing and Research Institute	Boras, Sweden
CSIRO	Sydney, Australia
Institute of Coal Chemistry	Shanxi, China
Technical University of Denmark	Lyngby, Denmark
Technische Universitat Graz	Graz, Austria
University of Stuttgart	Stuttgart, Germany
Imperial College	London, UK
University of Leeds	Leeds, UK
University of Newcastle	Callaghan, Australia
Monash University	Mulgrove, Australia
University of Kyoto	Kyoto, Japan
Kyushu University	Fukuoka, Japan
Hokkaido University	Sapporo, Japan
Tohoku University	Sendai, Japan
Åbo Akademi University	Turku, Finland
Ruhr Universität	Bochum, Germany
Universität Karlsruhe	Karlsruhe, Germany
Bandung Institute of Technology	Bandung, Indonesia
Swiss Federal Institute of Technology	Zurich, Switzerland
Technical University of Aachen	Aachen, Germany