# INTEGRATED FISCHER TROPSCH MODULAR PROCESS MODEL

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## ABSTRACT

With declining petroleum reserves, increased world demand, and unstable politics in some of the world's richest oil producing regions, the capability for the U.S. to produce synthetic liquid fuels from domestic resources is critical to national security and economic stability. Coal, biomass, natural gas, municipal solid waste, and other carbonaceous materials can be converted to liquid fuels using several conversion processes. The Fischer Tropsch (FT) process is a leading candidate for the production of liquid transportation fuels that operate with current engine designs and fit into the existing fuel distribution infrastructure [1]. Process configuration, component selection, and performance are interrelated and dependent on feedstock characteristics. This paper proposes a flexible modular approach to model an integrated FT process that utilizes a library of key component models in supporting kinetic data and materials and transport properties for allowing rapid development of custom integrated plant models. The modular construction will permit rapid assessment of alternative designs and feedstocks. The modeling approach consists of three thrust areas or "strands" – model/module development, integration of the model elements into an end to end integrated system model, and utilization of the model for plant design. Strand 1, model/module development, entails identifying, developing, and assembling a library of codes, user

blocks, and data for FT process unit operations for a custom feedstock and plant description. Strand 2, integration development, provides the framework for linking these component and subsystem models to form an integrated FT plant simulation. Strand 3, plant design, includes testing and validation of the comprehensive model and performing design evaluation analyses.

## INTRODUCTION

The objective of this effort is to develop a flexible integrated process model of the Fischer Tropsch (FT) process for synthetic fuels production plants. Process configuration, component selection, and plant performance are interrelated and dependent on feed properties. A robust comprehensive simulation tool using a modular approach supported by a library of fluid dynamic and kinetic based component and subsystem models, kinetic rates, and materials and transport properties would enable engineers to model a complete FT plant unique to the specific plant feed and product mix. The purpose of this work is to accelerate the design and deployment of FT or other synthetic fuels plants in the U.S. and to evaluate custom synthetic fuel plant designs for defense operations. This enhanced modeling capability will reduce risk, particularly during early commercialization where first of a kind design and new feedstocks will be used enabling more precise plant design. Once completed, the modeling project will provide a readily available tool that can be used for integrated plant design with technology evaluations and economic assessments. The integrated model will provide the capability to:

- Enable engineers to model a complete integrated FT plant and design the plant using more accurate scaling and performance predictions to achieve improved efficiency and safety and higher selectivity/productivity

- Select and evaluate process configuration and technology options based on the feedstock and products desired
- Virtually integrate new pieces of equipment and determine performance prior to building expensive prototypes
- Assess and optimize overall system performance
- Perform sensitivity studies based upon perturbations to the baseline design.

A modeling framework will be constructed with the ability to capture the complex interrelationships between unit operations required for feedstock gasification and conversion to synthesis gas (CO and $H_2$), synthesis gas cleanup and conditioning, catalytic reaction of the synthesis gas to liquid fuels, liquid product upgrading, and power generation. Figure 1 illustrates the overall process configuration and complexity associated with a synthetic fuels plant. The process can be divided into multiple sub-processes, each defined by its unit operations and process equipment components. Even in simplified detail, it is apparent that a complete synthetics fuels plant is complex and involves both process and thermal integration to achieve the overall system performance. The process model will provide a platform to model each unit operation to the level of sophistication and rigor necessary to accurately predict product stream chemistry; heat and mass transfer; fluid flow dynamics; multiphase separations involving gas, liquids, and solids; and plant economics.

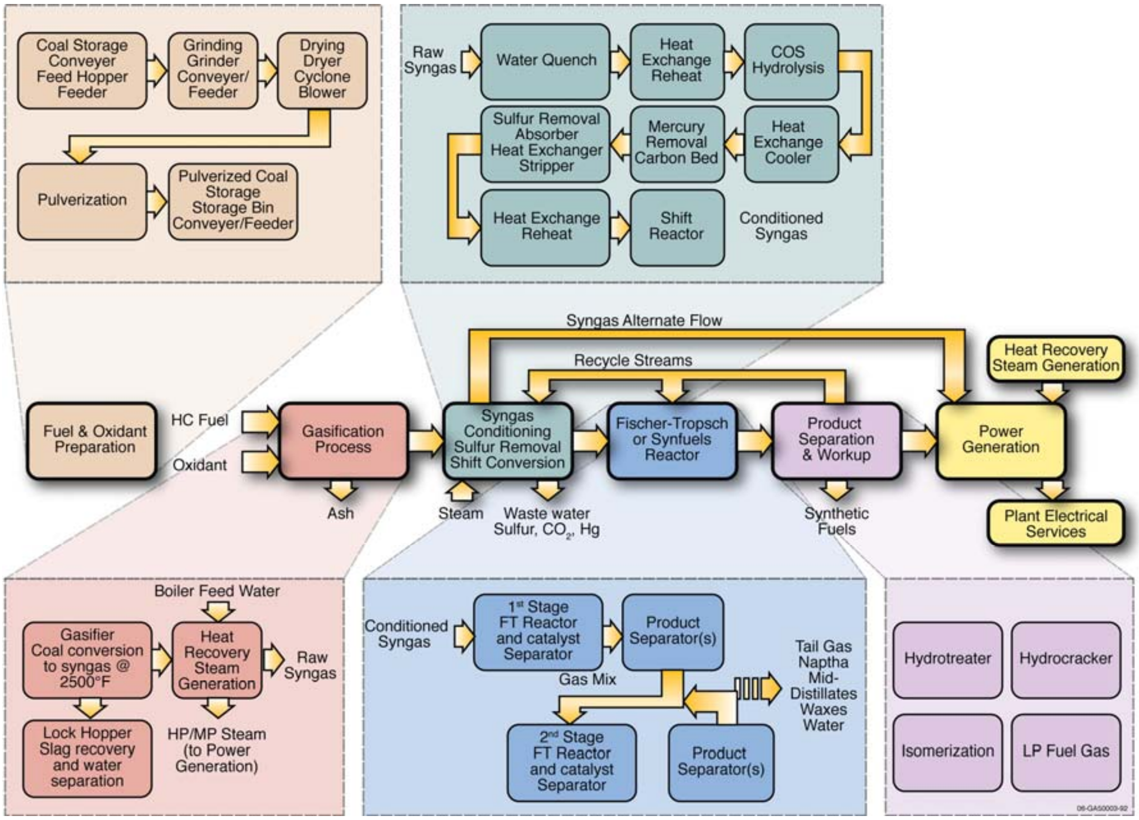

Figure 1. Block-flow diagram for a general reference synthetic fuels plant.

The products from this effort will be (1) an efficient computational tool to support rapid development of gasification-related synthetic fuels production plants, (2) the capability to perform plant design and economic assessments for industrial and defense applications, and (3) a virtual test bed to support operator training, plant control logical development, and front-end engineering design (FEED) studies.

## SIMULATION TOOL DEVELOPMENT APPROACH

A comprehensive computer tool capable of simulating the entire plant with detailed modeling of reaction-governed unit operations would be a tremendous aid in designing an efficient, economical, and robust plant. Such a tool would make it possible to rapidly reconfigure the plant in order to optimize specific objectives, such as synthesis gas composition, product distribution, power production, water use minimization, equipment configuration, plant layout, and emissions calculations. Since the integration of simulation models and predictive codes at this level of detail is inherently complex, several technical challenges must be addressed and resolved.

With an integrated approach, these models can be useful to guide the design process and provide more confidence in the governing mechanisms affecting the design goals (Figure 2). Assembly of the integrated simulation tool will build upon ongoing efforts at other institutions, such as for the FutureGen Power Plant [2]. The assembly process entails:

1. Identification, description, and documentation of unit operations and alternatives from front to back, including commercially proven and emerging technologies, such as:
    a. Feedstock assemblies, preparations, and feed alternatives (dry, slurry-feed, $CO_2$ slurries).
    b. Air separations units (including advancements in ion-transport membranes and pressure swing adsorption [PSA]).
    c. Commercially available gasifiers and gasifiers under development that are tailored for opportunity fuels (such as biomass, tires, and refuse-derived fuels), plasma gasifiers, steam reformers/pyrolysis gasifiers, fluid-bed gasifiers, and ultra-high temperature entrained flow gasifiers.

d. “Cold” and “hot” gas cleanup, shift reactors, and conditioning equipment, sulfur recovery, mercury removal, and $H_2/CO_2$ separation (PSA, cyrogenics, membranes, etc.).

e. Fixed-bed or slurry bubble column synthetic fuels reactors (FT and others), with all appurtenant equipment items.

f. Product refining and upgrade unit operations (hydrotreating, hydrocracking, isomerization, distillation, etc.).

g. Power generation gas turbines, steam turbines, fuel cells, and reciprocating engines.

h. Heat recovery steam generators, fired boilers, etc.

2. Identification and development of database libraries for feedstock and product stream properties, reaction rate data, economic data, materials physical and mechanical properties, and discharge/emissions regulations, including but not limited to the following:

a. Thermodynamic (heat capacity, heat of formation, free energies, etc.), transport property data (viscosity, diffusivity), feedstock elemental and trace element analysis, and proximate analyses and heating values/heats of formation.

b. Kinetic data and rate expressions for constituent reaction, including devolatilization, char-oxidation, char gasification, gas-phase homogeneous reactions, catalytic surface reactions, hydrotreating, hydrocracking, isomerization, esterification, etc.

   c. Catalyst properties, conversion data, chain-growth factors, particle size and density, surface area, pore volume and interstitial space, attrition factors, corrosion, poisoning susceptibility rates, etc.

   d. Adsorption column and sorbent bed particle parameters (e.g., interfacial area, mass transfer coefficients, binary and ternary diffusion coefficients, column flooding and pressure drop correlations, sorbent particle size, reactivity and reaction rates, etc.).

   e. Materials properties for high-temperature, high-pressure service (e.g., corrosion data, yield strength, tensile strength and modulus of elasticity and elongation, density, thermal expansion coefficients, etc.).

   f. Feedstock and commodity price details, including materials costs for piping, vessels, electrical, instrumentation, etc.

   g. Emissions regulations based on geographical location.

3. Identification and assembly of commercial software packages, custom codes, and algorithms for prediction of reaction behavior and performance of select gasifiers, synthesis gas cleanup separations columns, FT reactors, and gas turbines. This includes computational fluid dynamics (CFD) codes for gasifiers, fixed-bed gasifier models, fluidized-bed gasifier codes, gas scrubbing and stripping codes, CFD codes for multiphase gas-liquids-solid reactors [3,4] and gas turbine codes.

4. Development of routines to read database libraries to assemble case-specific reaction expressions.

5. Development of a generalized economics model to calculate plant pro forma cost and revenue macroeconomics.

6. Identification, evaluation, implementation, and new development of a code integration framework (controller) to rapidly link and wrap multiple custom codes with a process simulation package and the database library to create an integrated plant process model.

7. Identification, evaluation, and adoption of high-fidelity/high-efficiency solvers to utilize multilevel computer work stations, computer clusters, and supercomputers to rapidly and accurately converge the integrated system of codes representing the plant.

8. Identification, evaluation, adoption, and development of graphical user interfaces to plot, visualize, and interpret simulation solutions and results.

9. Identification, evaluation, adoption, and development of graphical tools for virtual depiction and user interface with process modules for the purpose of efficient plant design, operator training, and interactive sensitivity analysis and transient behavior studies.

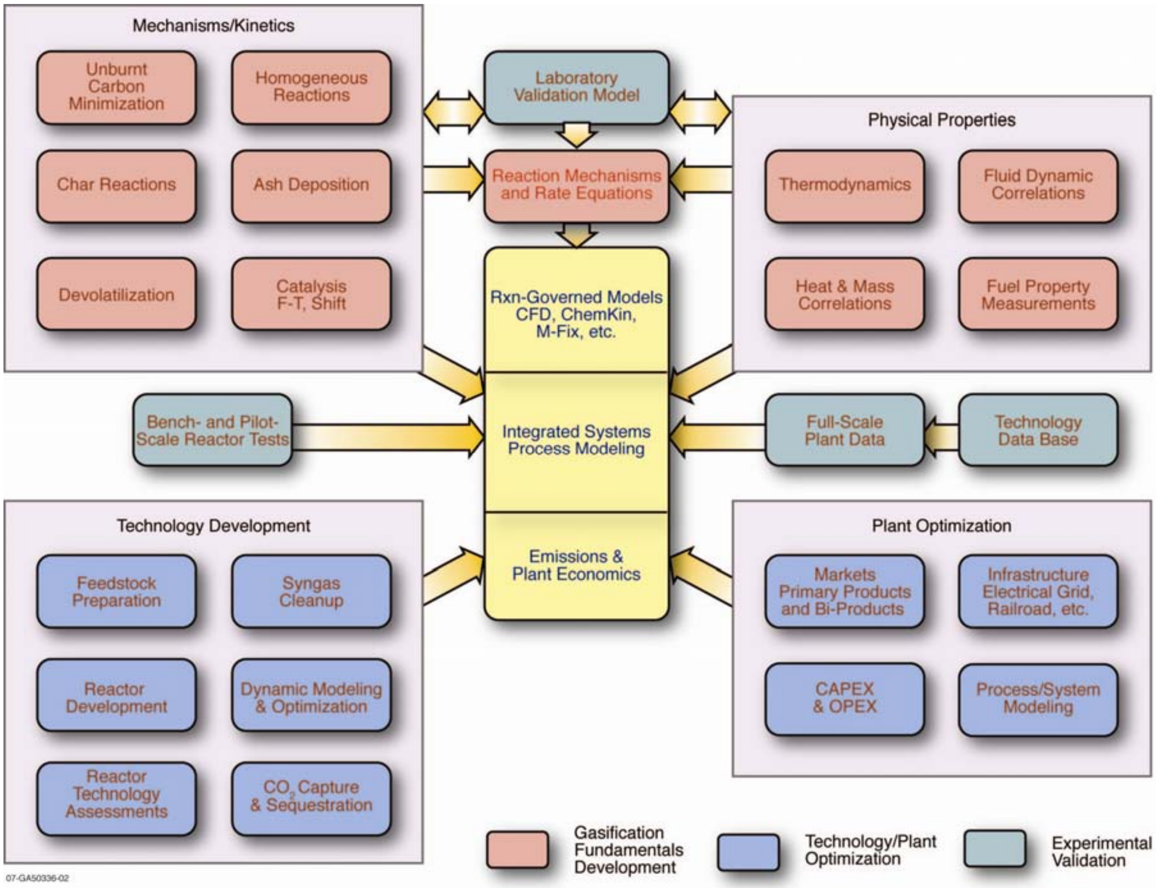

Figure 2. Elements factoring into complete process model.

## SIMULATION ARCHITECTURE

Three “strands” define this project: (1) model/module development including component and properties data libraries, (2) integration development, and (3) plant design/model validation. Strand 1, model/module development, entails identifying, developing, and assembling a library of codes, user blocks, properties data libraries, and data for FT process operations for a custom feedstock and plant description. Strand 2, integration development, provides the Virtual Engineering Framework (VEF) for plugging detailed models into the FT plant simulation. Strand 3, plant design, includes testing and validation of the comprehensive model and performing design evaluation analyses.

The integrated simulation capability links a hierarchy of plant- and equipment-level models with varying levels of fidelity and computational speed suitable for either preliminary conceptual design or detailed final design. The backbone of the simulation tool will consist of an FT process model augmented with specific component models to customize the plant design. Connected to the front/back ends of the FT process model are:

- Self-contained models of the gasifier, acid gas removal system, turbines, product upgrading, and FT reactor
- Library of key component models, supporting data and transport properties
- Reduced order models (ROMs) or pre-computed solutions from computational fluid dynamics analyses.

Figure 3 illustrates the database and reactions code feeding into the process model. Component models will then be incorporated into the process model or converted into ROMs when necessary and sufficient for specific accuracy and/or efficiency requirements. ROMs for the gasifier and FT reactor can reduce the computational time required for complex simulations and provide interfaces that allow for integration with plant simulations. This reduction can be accomplished by developing a low-order model based on mathematical techniques, such as multiple linear or non-linear regression, proper orthogonal decomposition, network-of-zones [5] or artificial neural networks [6]. In some cases, it will be acceptable to call pre-computed solutions or to use data tables to provide an expert (or advisory) solution using tabulated experimental, pilot plant, or full-scale data. Artificial intelligence solutions typically require extensive test data and methods of interpolating the databases.

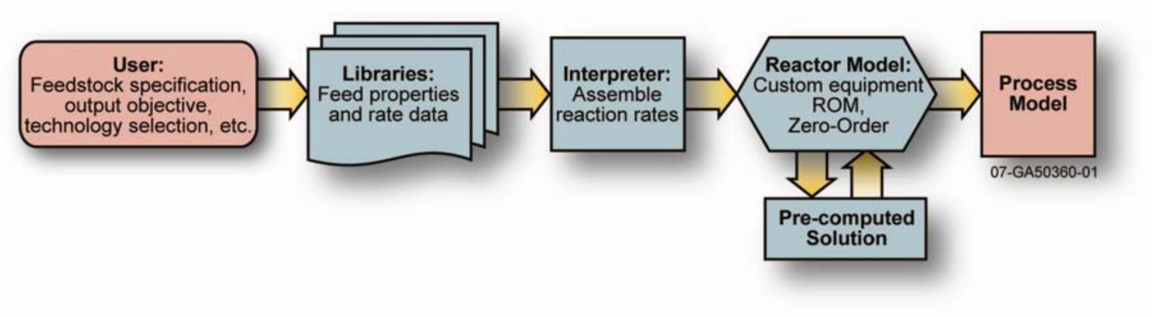

Figure 3. Illustration of database and reactions code feeding into process model.

The VE Suite VEF [7] will include a hierarchy of models and visualization tools to construct, perform, and interrogate simulation results for component models and overall plant performance at multiple levels of detail within a three-dimensional, user-centered, interactive environment [8]. The VEF will enable engineers to better understand the interactions of different equipment components and to identify weaknesses and processes needing improvement.

## SUMMARY

The integrated simulation tool described herein will enable engineers to effectively design and simulate gasification-related synthetic fuel production plants. This paper outlines the authors' vision for an integrated simulation environment, represented by Figure 4, is comprised of a set of specialized models, which provide the opportunity to improve plant performance and economics. Engineering class simulations can be conducted for controls operability and operator training. This is, admittedly, an ambitious task which will require many man-years of effort to complete. The results of this work can provide a valuable tool to accelerate the deployment of synthetic fuels plants and enable independent technology evaluations and assessments of custom plant configurations.

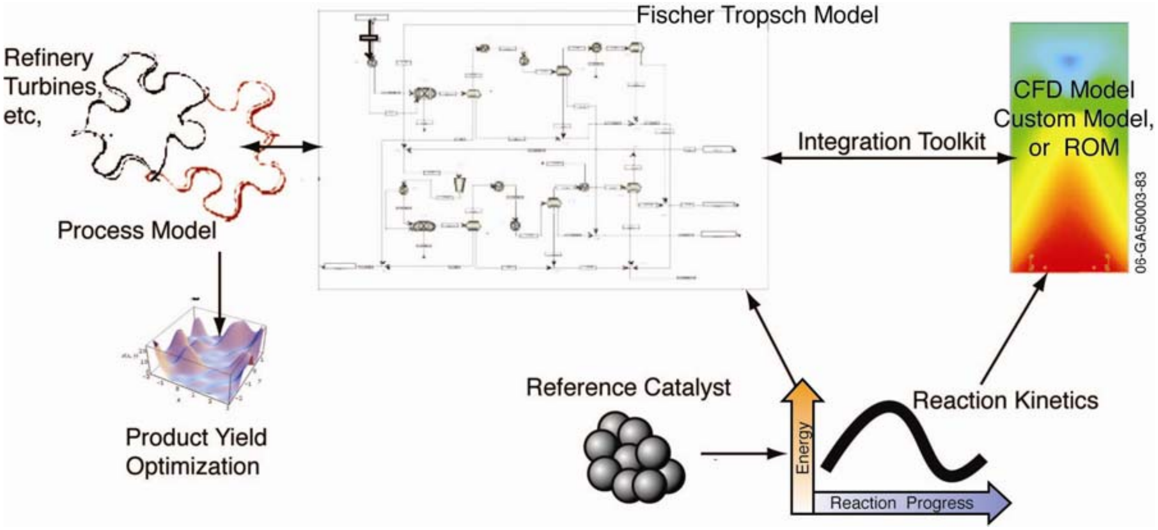

Figure 4. Vision of integrated simulation environment.

## REFERENCES

1. Steynberg, A.P., and Dry, M.E., Fischer-Tropsch Technology, Studies in Surface Science and Catalysis, Vol. 152, Elsevier, 2004.

2. Zitney, S.E., et al., “Advanced Process Co-Simulation of the FutureGen Power Plant,” *The Clearwater Coal Conference, 31st International Technical Conference on Coal Utilization and Fuel Systems*, Clearwater, FL, May 21-25, 2006.

3. Troshko, A.A. “CFD Modeling of Slurry Bubble Column Reactor for Fischer-Tropsch Synthesis,” *AIChE 2006 Annual Meeting*, San Francisco, CA, November 12-17, 2006.

4. Antal, S.P., Lahey, Jr., R.T., and Al-Dahhan, M.H. “Simulating Churn-Turbulent Flows in a Bubble Column using a Three Field, Two-Fluid Model,” Paper No. 182, *5th International Conference on Multiphase Flow*, ICMF’04 Yokohama, Japan, May 30–June 4, 2004.

5. Bezzo, F., Macchietto, S., and Pantelides, C.C., “A General Methodology for Hybrid Multizonal/CFD Models Part I. Theoretical Framework,” *Computers and Chemical Engineering*, Volume 28, 2004, p. 501-511.

6. Shaikh, A. and Al-Dahhan, M.H., “Development of an Artificial Neural Network Correlation for Prediction of Overall Gas Holdup in Bubble Column Reactors,” *Chemical Engineering and Processing*, Volume 42, Number 8, August 2003, pp. 599-610(12).

7. Xiao A.R., Bryden, K.M., and McCorkle, D.S.,” VE-Suite: A Software Framework for Design-Analysis Integration during Product Realization,” *Proceedings of the ASME International Design Engineering Technical Conferences and Computers and Information in Engineering Conference*, Volume 3, Pts A and B, 2005, p 859-867.

8. McCorkel, D.S., et al., “Towards the Integration of APECS with VE-Suite to Create a Comprehensive Virtual Engineering Environment,” *The Clearwater Coal Conference, 32nd International Technical Conference on Coal Utilization and Fuel Systems*, Clearwater, FL, June 10-15, 2007.