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Computational Fluid Dynamic Applications

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DISCLAIMER

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ABSTRACT

The rapid advancement of computational capability including speed and memory size has prompted the wide use of computational fluid dynamics (CFD) codes to simulate complex flow systems. CFD simulations are used to study the operating problems encountered in system, to evaluate the impacts of operation/design parameters on the performance of a system, and to investigate novel design concepts. CFD codes are generally developed based on the conservation laws of mass, momentum, and energy that govern the characteristics of a flow. The governing equations are simplified and discretized for a selected computational grid system. Numerical methods are selected to simplify and calculate approximate flow properties. For turbulent, reacting, and multiphase flow systems the complex processes relating to these aspects of the flow, i.e., turbulent diffusion, combustion kinetics, interfacial drag and heat and mass transfer, etc., are described in mathematical models, based on a combination of fundamental physics and empirical data, that are incorporated into the code. CFD simulation has been applied to a large variety of practical and industrial scale flow systems.

Keywords: CFD, Fluid Dynamics, Heat Transfer, Combustion, Multiphase, Industrial Applications

Nomenclature:

C_k	coke species
C_{pj}	specific heat of species j (J/kg/K)
fj	concentration of species j
h	enthalpy (J/kg)
Mj	molecular weight of species j
p	pressure (Pa)
Pj	gaseous species j
R	universal gas constant
S_ξ	the sum of source terms
T	temperature (K)
u_i	velocity component (m/s)
x_i	coordinate (m)

Greek Symbols

ρ	density (kg/m^3)
ξ	general gas flow property
θ	gas volume fraction
Γ	effective diffusivity

Subscript

o	reference
i	direction index
j	species index
k	droplet/particle size group

INTRODUCTION

Energy has been widely used for heating, transportation, and producing goods to improve the quality of life, i.e., comfortable living environment, convenient mobility, and easy communication. But the use of energy also created environmental pollution problems, such as acid rain, smog, etc. While public demand for energy, both direct and indirect, in products produced by industry, has increased tremendously over the last century, public demand and government mandates for energy conversion systems with higher efficiency and lower pollutant emission have also increased greatly since the 1960's. To accomplish these goals, a greatly increased understanding of the detailed physics and interaction of parameters governing the operation of these systems is required.

In the past, experiments and tests were the primary sources of the information on the operation of an energy conversion system that could be analyzed to improve understanding of the system. Experimental and testing program are usually both very costly and time consuming. In the early 1960s, NASA started to develop computational fluid dynamic (CFD) codes to aid the development of the rocket and space programs. Later, national laboratories developed various CFD codes for their nuclear and military programs. Since computer speed and memory capabilities have increased dramatically, reducing cost, the use of CFD codes in a variety of industrial applications has been increasing significantly in recent years.

A CFD calculation can be used in industry for the following purposes: 1) Trouble Shooting: A CFD code calculates the detailed local flow properties of a flow system to identify local regions where a problem exists. The information can be used to help train a novice operator to better understand the system. It can also be instrumental for investigating overall system problems and developing solutions to these problems; 2) Parametric Analysis: A validated CFD code for a specific application is set up for a large number of calculations in a short time with a minimal cost. A parametric analysis, or a set of computational experiments, is constructed to investigate the impact of different operating and design conditions on the performance of the system. The analysis is valuable in helping an experienced system operator further improve plant performance; 3) Performance Optimization: A parametric analysis generally leads to opportunities for optimization. Based on the results of the parametric analysis, control schemes are developed to adjust the operating parameters; which thus, optimize the performance of the system; 4) Conceptual Design: A CFD code is also be used to explore innovative concepts for improving the performance of a system before the plant is built - at the design phase.

Since the topic of CFD applications is so broad, a detailed survey of all the works is not intended here. This paper describes only the CFD applications that the authors have been experienced in over the past twenty years. The paper is divided into two major parts. The first part introduces general concepts of CFD development. The second part briefly presents various CFD applications, including glass furnaces, magnetohydrodynamic power generation systems, internal combustion engines, fluidized bed combustors, and gas turbines.

GENEREAL CFD CONCEPTS

A CFD code is developed to characterize the physics and chemistry if reaction is present of a flow system of interest. The development of a CFD code includes several steps as illustrated by the flowchart in Figure 1. First, the flow characteristics of the system need to be carefully examined so that appropriate assumptions can be made. Based on the assumptions, fluid components (gas species, liquid droplets, and/or particles) and flow properties that determine the system state (velocity, temperature, pressure, etc.) are identified and the governing equations of these flow properties are be derived from the conservation laws of mass, momentum, and energy. Complex flow phenomena, such as turbulent mixing, chemical reactions, radiation heat transfer, and interfacial interactions, are generally included by developing simplified phenomenological models based on a mixture of fundamental physics and correlations derived from experiments.

The governing equations are primarily non-linear coupled partial differential equations. Even with the simplified models, an analytical solution of these equations is impossible to obtain. Further simplifications are required. The governing equations are converted to algebraic equations on a discretized grid system. The algebraic equations for flow properties are non-linear and coupled and an exact solution of these equations is still out of reach. Therefore, various iterative routines are selected to find approximate solutions of these algebraic equations. The iterative routines require such a large number of calculations that a computer is the necessary for the task. Again, the discretized algebraic equations and solution iteration scheme are converted and coded into computer language, usually FORTRAN. Because computers only carry along a finite number of significant digits in computations, round off error and loss of precision due to truncation must be carefully controlled in the computational schemes. Typically, tens of thousands lines of computer code are needed to convert the discretized algebraic equations and the iterative solution routines. The collection of lines computer code is called a CFD code. Many programming bugs, i.e., typographical errors, formulation mistakes, unit inconsistency, and numerically unstable computation algorithms may exist in a CFD new code. A debugging process is required to find the bugs, fix the mistakes, and improve the numerical stability of the computations. In authors' experience, the debugging and improvement work is never done as long as you are using a CFD code and applying it to new systems or new operating conditions.

An iterative routine is implemented to run the code to obtain a converged result. Since a converged numerical result is not an analytical solution of the governing equations of the flow system, verifications with other numerical results and validations against test data are definitely needed before a CFD code can be used to simulate a flow system. A CFD code is in principle applicable to any flow system. However, a CFD calculation with many flow features is usually very unforgiving in terms of numerical stability when computing flow systems operating near the physical limits of the system (often true for industrial systems) or when computing the solution in regions where steep gradients exits due to the non-linear nature of governing equations. Due to these difficulties generic CFD codes often have convergence problems when applied to

specific industrial applications. A more practical approach is to develop a solid generic base CFD code for a simple flow systems and then to modify this code with specific models or computational techniques to handle the specific complex processes in practical flow systems when the application changes.

In the following sections, a CFD code developed for the simulation of fluid catalytic cracking (FCC) riser reactors [1] will be used as an example to elaborate the aforementioned CFD code development steps.

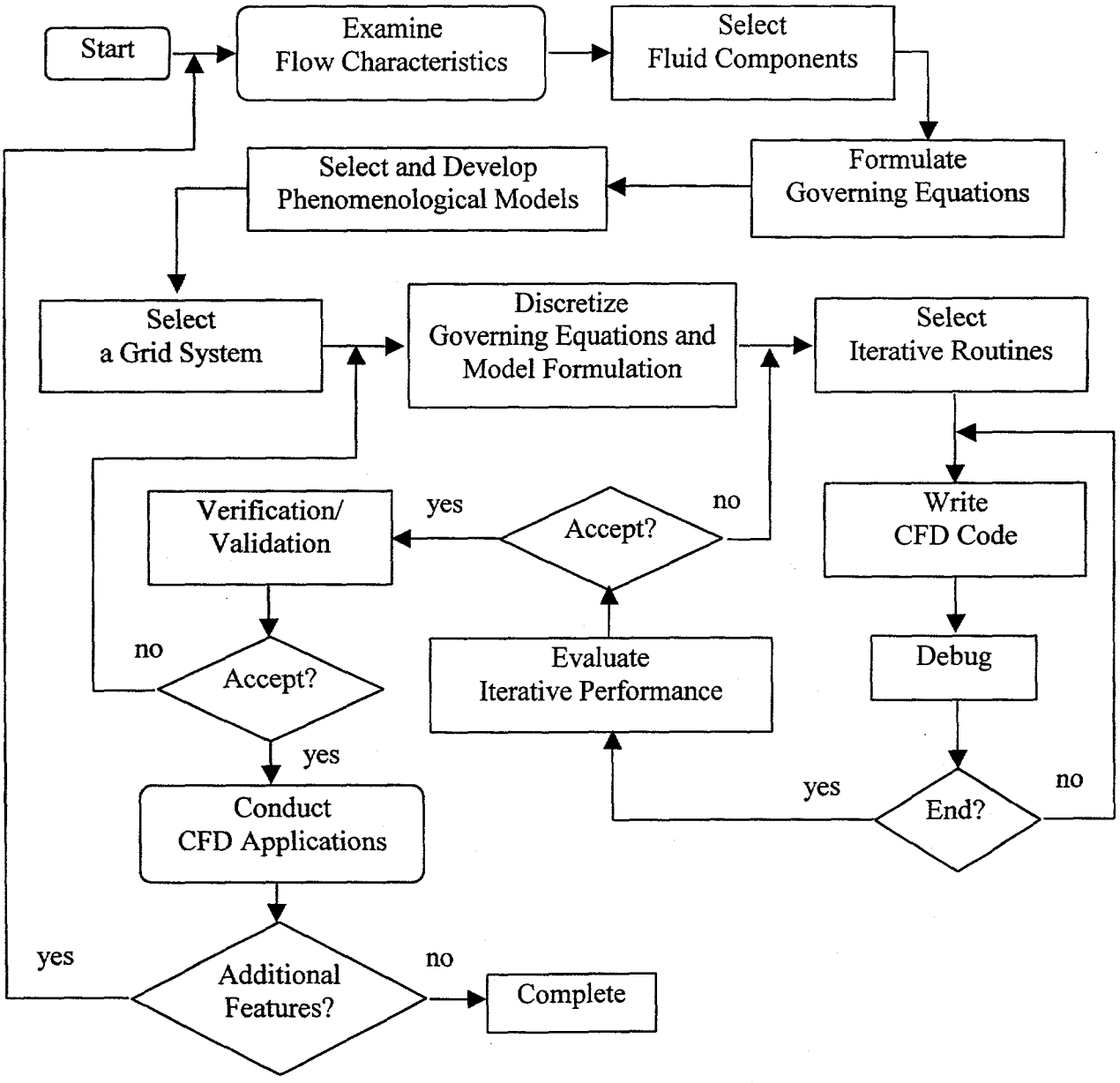


Figure 1 A Flowchart of CFD Code Development

Flow Characteristics

FCC technology was developed in 1940s. Since then, it has become the refinery industry's most important process to convert crude oil to more valuable products such as gasoline. Today, the FCC units in U.S. refineries produce about 40% of the nation's gasoline pool. In a modern FCC unit, it is essential to optimize product selectivity for feed types. Recently, refineries have become interested in improving the of the feed injection system and the development of short residence time riser units [2]. To facilitate and speed up the development of new and/or upgraded FCC systems, detailed knowledge of the relationships between process operating parameters and conditions within the system is needed. Such knowledge can be obtained by using a CFD code that is validated by the experimental measurements from test units.

A typical FCC unit includes three major components: a riser reactor, a stripper/separator, and a regenerator. Figure 2 shows a simple sketch of a FCC unit. A spray of feed oil is injected into the riser to be converted to lighter oil products. Catalyst particles that are used to vaporize oil droplets and enhance the conversion process are transported to the bottom of the riser reactor from a regenerator. A small amount of inert gas is needed to lift particles in the entrance region of the riser. Oil droplets are vaporized when heated to the boiling point. Then, oil vapor is cracked into various lighter oil products via the catalyst and heat. Coke is a by-product of the cracking processes, and it deposits on the catalyst surface. Coke deposition lowers the activity of catalyst particles. The end of the riser is connected to a separator, in which oil products and spent catalyst particles (covered with coke) are separated. Oil products are sent to a distillation column for further processing, and the spent particles are transported to the regenerator in which the coke deposit is burned off with air. After burning off the coke deposit, the heated catalyst particles regain the catalytic activity. The regenerated catalyst is then recycled back to the riser reactor for reuse in the cracking process. At present, the flow simulation focuses on the multiphase, reacting riser flow.

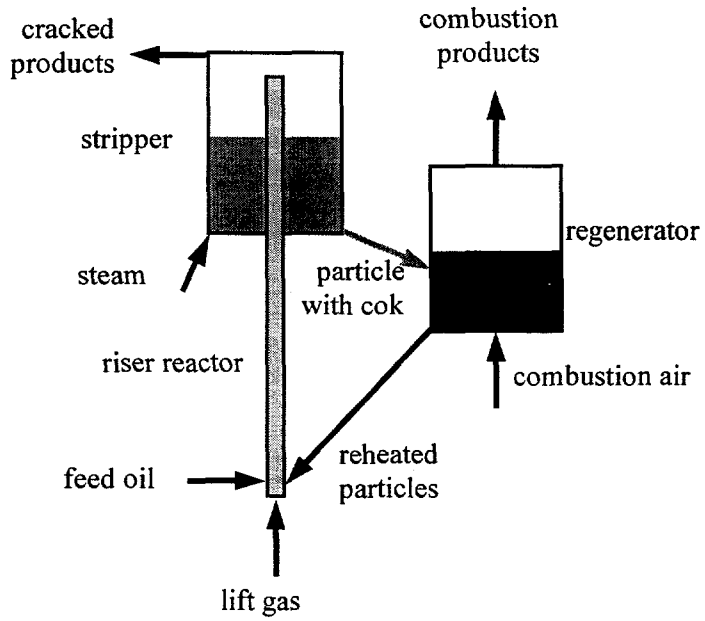


Figure 2 A Typical FCC Unit

In a riser, there are three major processes: mixing, vaporization, and cracking reactions. Mixing encompasses the combined effects of interfacial interactions (momentum and heat transfer between phases), flow convection and turbulent diffusion of gas, oil droplets, and catalyst particles. During the mixing process, the heat carried by the catalyst particles is transferred to the gas and the oil droplets. Generally, the catalyst is heated up to a temperature much higher than the boiling point of the feed oil, and the catalyst mass flow is much larger than the oil flow. Consequently, the vaporization process is controlled by the heat transfer rate to oil droplets. During vaporization, a liquid oil droplet releases oil vapor in the presence of hot catalyst particles. Following vaporization, cracking takes place. Feed oil vapor contacts catalyst particles, and the cracking reactions on the catalyst surface convert the feed oil vapor to numerous light oil species and dry gas. Coke is a by-product of the process.

Gas-liquid-solid interactions in an FCC unit are among the most interesting and difficult areas of study for the development of advanced FCC systems. A multi-phase, multi-species, turbulent reacting flow simulation code was specifically written for the simulation of such an FCC riser flow. The code is called the Integral CracKing FLOw Simulation, or ICRKFLO.

Formulation of the Multiphase, Reacting Flow Governing Equations

The cracking reactions in an FCC system involve thousands of oil species [3]. Several numerical stiffness problems are expected if all the oil species and the cracking reactions are included in a flow computation directly. Instead, ICRKFLO uses an alternative approach by dividing the flow computation into two steps: (1) a flow calculation with a highly reduced reaction mechanism and a limited number of lumped species and (2) a detailed kinetics calculation based on the pre-calculated flow field. By assuming that the majority of the reaction species have little impact on the flow field, the first-step flow calculation includes only a few lumped species to account for the impact of density change and heat transfer due to reactions. By de-coupling the highly detailed kinetic calculations from the feed back of the pressure-velocity field, the second-step kinetics calculation becomes very stable numerically and tens or hundreds of reacting subspecies can be included in the calculation.

Fluid Components

The flow calculation considers the fluid components in an FCC riser flow, including major gaseous species, liquid droplets, and catalyst particles. To formulate the governing equations of the flow, an Eulerian approach assumes that gaseous species, liquid droplets and catalyst particles are all continua in the flow.

A reduced 4-lump kinetic model [4] is used to represent the major cracking reactions in the first-step flow calculation. The reduced kinetic model includes two cracking reactions with four lumped oil components: three gaseous species (feed oil, light oil, and dry gas) and one solid by-product (coke). These oil lumps are arbitrarily defined as follows. Feed oil (P_1) consists of those oil species of a boiling point higher than 500 K. Light oil (P_2) includes those species with a boiling point lower than 500 K and a carbon number higher than 5. Dry gas (P_3) includes oil vapor of carbon number C_5 and below. Coke (C_k) is mostly carbon. Carrier (P_4) and lift gas (P_5) species not involved in the reactions are also included in the gas flow calculation. A more detailed kinetic model is used in the second-step kinetic calculation. In this step, many more species (referred as subspecies in the following discussion) are considered.

In an FCC unit, feed oil is injected into the riser in sprays and catalyst particles are transported into the riser by carrier and lift gases. The Eulerian approach divides oil droplets and

catalyst particles into groups by sizes and treats the number density of droplets/particles of a size group as continuous property of the flow.

Governing Equations

Flow is governed by the equations of state and the conservation laws of mass, momentum, and energy, from which governing equations can be derived. The flow properties needed to determine the state of this flow system and to evaluate its performance are pressure p, density ρ, temperature T, enthalpy h, species concentration f_i, and velocity components u_i, i=1,3 for gas phase and number density n_k, temperature T_k, and velocities $u_{k,i}$, i=1,3, for the k^{th} droplet/particle size group.

Equations of State

Assuming gas species can be treated as an ideal gas mixture, the state equations include the ideal gas equation (1) and the caloric equation (2).

$$p = \rho RT \sum_{j=species} \left(\frac{f_j}{M_j} \right) \tag{1}$$

$$h = \sum_{j=species} f_j C_{p_j} (T - T_o) \tag{2}$$

In the equation (1), R is the universal gas constant and M_j is molecular weight of species j. In the equation (2), C_{pj} is the specific heat of species j and T_o is a reference temperature.

Conservation Equations

The gas phase conservation equations include the continuity, momentum, energy, and species equations. These equations can be expressed in a common form:

$$\sum_{i=1}^{3} \frac{\partial}{\partial x_i} (\theta \rho u_i \xi - \Gamma_\xi \frac{\partial \xi}{\partial x_i}) = S_\xi \tag{3}$$

in which ξ is a general gas flow property, x_i are coordinates, θ is gas volume fraction, Γ is effective diffusivity, and S_ξ is the sum of source terms. The effective diffusivity including both laminar and turbulent viscosities and the source terms are discussed in the phenomenological models section. The general gas flow property is a constant 1 for the continuity equation, u_i for the x_i-momentum equation, h for the energy equation, and f_j for the species equations.

For k^{th} size group of the droplet/particle phase, the conservation equations of mass, momentum, and energy are expressed in a common form:

$$\sum_{i=1}^{3} \frac{\partial}{\partial x_i} (n_{d,k} u_{d,k,j} \xi - \Gamma_\xi \frac{\partial n_{d,k} \xi}{\partial x_i}) = S_\xi \tag{4}$$

in which ξ is a general droplet/particle property, Γ is the droplet/particle diffusivity resulting from interaction with turbulence in the gas phase, and S_ξ is the sum of source terms. A special particle property for the FCC flow simulation is the coke concentration C_k. Coke generated from the cracking reactions precipitates on the surface of catalyst particles. A coke transport equation similar to Eq. (4) is derived. The general droplet/particle flow property is a constant 1 for the number density equation, $u_{k,j}$ for the momentum equation, T_k for the energy equation, and C_k for the coke equation.

Phenomenological Models

The effective diffusivity in the conservation equations is calculated from both laminar and turbulent viscosities. Laminar viscosity is a fluid property and turbulent viscosity needs to be determined from a multi-phase k-ε turbulence model. The source terms of the governing equations are generally derived from phenomenological models. The continuity equation has a source term accounting for droplet evaporation. The evaporation rate is calculated from a spray evaporation model. The species equations include source terms for species consumption/generation. The species consumption/generation rates can be derived using a time-integral lumped kinetic model. The momentum equations include source terms for the remaining viscous stress terms, drag forces between phases and momentum added or removed due to mass transfer between phases. The energy equations include source terms for the heat transfer between phases and heat of reaction in the gas phase. The drag forces and heat transfer rates are calculated from an interfacial interactions model. The particle flow is one of the most interesting and difficult to model because particle collisions are frequent and they tend to redistribute the particles in the flow. A particle-solid (particle-particle and particle-wall) interaction model was required to properly characterize the dense particle flow. These models are briefly presented in the following. More details of these models could be found in previous publications [1,5].

Multi-phase k-ε Turbulent Model

A turbulent flow consists of a spectrum of rotational eddies. The eddies, having a size ranging from a tiny, dissipative sized rotation to one the size of the flow, can effectively transport and mix species, momentum, heat, and other transportable components or properties of the flow. The mixing rates of the turbulent motion are generally several orders of magnitude greater than those of the molecular diffusion. Launder and Spalding [6] developed a turbulence model employing the turbulent kinetic energy k and its dissipation rate ε for single-phase flows. Two additional transport equations, like Eq.(4), for these turbulent parameters were introduced. By solving these two transport equations, the turbulent diffusivity can be determined from the values of k and ε. Among others, Zhou and Chiu [7] later modified the turbulence model for multi-phase flows and an enhanced version of their model is used in the ICRKFLO code.

Spray Evaporation Model

Liquid feed oil needs to be vaporized so the oil vapor may be cracked into products. A spray model that empirically correlates droplet size, velocity, and spray angle with the injector size and injection pressure [8] can be used to determine the droplet inflow conditions for the flow simulation. Once the droplets enter the reactor, the heating and the vaporization of the droplets starts to occur. A droplet vaporization model was based on the fundamental physics of stationary single droplet vaporization and then modified for large groups of droplets in a connective environment [9]. The vaporization rate is derived as a function of droplet size, temperature and velocity differences between droplets and gas, and latent heat.

Time-Integral Lumped Cracking Model

The lumped cracking model was developed based on the 4-lump cracking kinetics model [4] and the integral reacting-flow time-scale-conversion method [10]. The kinetic model considers two reactions: (a) feed oil is converted to light oil, dry gas, and coke; and (b) light oil is further converted to dry gas and coke. Many reacting flow calculations using a differential approach to calculate reaction rates experience severe numerical stiffness problems due to the difference of the flow and the reaction time scales. A time scale integral approach was developed to overcome these numerical problems. The kinetic model is used to determine the consumption rate for the feed oil species, and the generation rates for light oil, dry gas, and coke.

Interfacial Interaction Models

Interfacial interactions include the exchanges of momentum and energy between phases. In the dilute flow region, oil droplets and catalyst particles are driven mainly by the drag force from the gas flow. An empirical Reynolds formula correlating the drag force with local flow properties and velocity difference is used to calculate the interfacial drag force. The source terms of drag forces are used in the gas, liquid, and solid momentum equations. Catalyst particles are the principal heat carriers, supplying energy to vaporize the oil droplets and crack the heavy oil species into gasoline and other lighter products. An empirical Nusselt formula is used to calculate the heat transfer between particles and gases, and between droplets and gas. The source terms of heat transfer rates are used in the gas, liquid, and solid energy equations.

Particle-Solid Interaction Models

FCC riser reactor has dense flow region where moving particles tend to collide with neighboring particles frequently and the collisions cause the particles to diffuse across the flow stream. Particle diffusivity is derived from the collision frequency among the particles. In addition, a solid shear stress term is derived to account for the momentum loss due to the collisions between particles and the wall. In some region of the FCC flow, particles are directly in contact with the neighboring particles or packed. Particles exert solid pressure on other particles. Lyczkowski et. al. [11] assumed that the solid pressure is a function of local solid volume fraction when solid fraction exceeds a packed value. The source terms of particle diffusivity, particle shear stress, and solid pressure are part of the particle momentum equation.

Subspecies Kinetics Calculation

The major gaseous species in the above-mentioned reacting flow calculation are lumped into broad categories: feed oil, light oil, and dry gas. However, within these oil species lumps exist a very large number of oil subspecies produced from numerous kinetic reactions in the riser. These subspecies are not solved in the first-step flow calculation to avoid numerical stiffness problems. After the first-step calculation, the transport equations of these kinetic subspecies can be solved on the pre-determined flow field. Free from the interactions with numerical fluctuation of the pressure and velocity during iteration, the calculation of the partially de-coupled species transport equations becomes very stable numerically. A more detailed description of the second step subspecies calculation is given in [12].

Computational Methods

The governing equations, Eqs.(1)-(4) must be solved for specified boundary conditions. Since analytical solution for the partial differential equations (3) and (4) is not available, an approximate numerical solution algorithm is used. ICRKFLO uses a control volume approach to convert the governing equations to algebraic equations on a discretized grid system.

Computational Grid System

A Cartesian coordinate system and a staggered grid system are used in the numerical solution algorithm. A computational grid is defined on a Cartesian coordinate system by dividing the space into smaller computational nodes. Figure 3 shows a simple x-y grid and an illustration of a staggered grid system. In the figure, a computational node is represented by its indices (i,j,k) instead of the dimensions x, y, and z, the arrows represent the nodes that are used to calculate gas phase momentum equations and the circles represent the nodes that are used to calculate all the other flow properties. Some of the computational nodes can be blocked so the

fluid would not flow through the node as shown as a triangle in Fig.3. The blocked node techniques can be used to construct a complex flow field with the simple Cartesian coordinate system. The computational domain can also be divided into several sections. Flow computation is performed at each section and the computed flow information exchanges only on the interface of the neighboring sections.

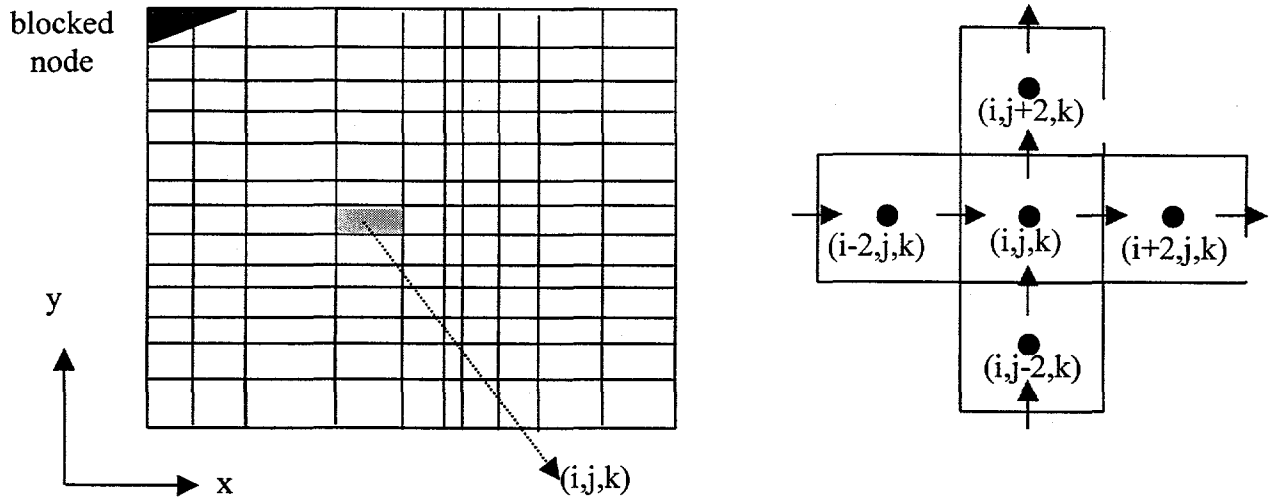


Figure 3 Representation of Staggered Grid System

The governing differential equations can be converted to algebraic equations on a computational grid system by various discretization methods. The control volume approach treats a computational node as a control volume (cell) and assumes the flow properties in a cell are uniform. Considering an equation governing ξ at a node (i,j,k), the equation can be integrated over the control volume to yield an algebraic equation.

$$A_p(i,j,k)\xi(i,j,k) + A_{s,-1}(i,j,k)\xi(i-1,j,k) + A_{s,+1}(i,j,k)\xi(i+1,j,k)$$

$$+ A_{s,-2}(i,j,k)\xi(i,j-1,k) + A_{s,+2}(i,j,k)\xi(i,j+1,k)$$

$$+ A_{s,-3}(i,j,k)\xi(i,j,k-1) + A_{s,+3}(i,j,k)\xi(i,j,k+1) = B_s(i,j,k) \qquad (5)$$

in which ξ is the unknown flow property, A_p and A_s are coefficients associated with convective and diffusive terms, and B_s is related to the source terms of the governing equation. Because the governing equations are mostly nonlinear, the coefficients and constant term in the equation (5) could also contain the unknown flow property. In this case coefficients and constant term are calculated from the current estimate of the unknown for an iteration step in the solution cycle.

Iteration Routines

For a typical FCC riser flow simulation, there are more than forty governing differential equations and tens or hundreds of thousands of computational nodes. Thus, the number of algebraic equations to be solved quickly added up to more than a million. Therefore, efficient iteration routines are needed to find a numerical solution.

ICKFLO use two layers of iteration routines: a low level solver for a single flow property variable, and an overall iteration routine for all flow property variables as shown in Figure 4. The low lever solver solves for one flow property variable at a time while keeping the other flow variables constant. The low level solver has three iteration loops in three coordinate directions. When only a row of nodes is considered, the equations of these nodes can be solved with a tridiagonal elimination method. The overall iteration routine solves flow property variables in the gas, liquid, and particle loops. Patankar's SIMPLER scheme [13] is used to solve the gas phase pressure linked momentum and continuity equations.

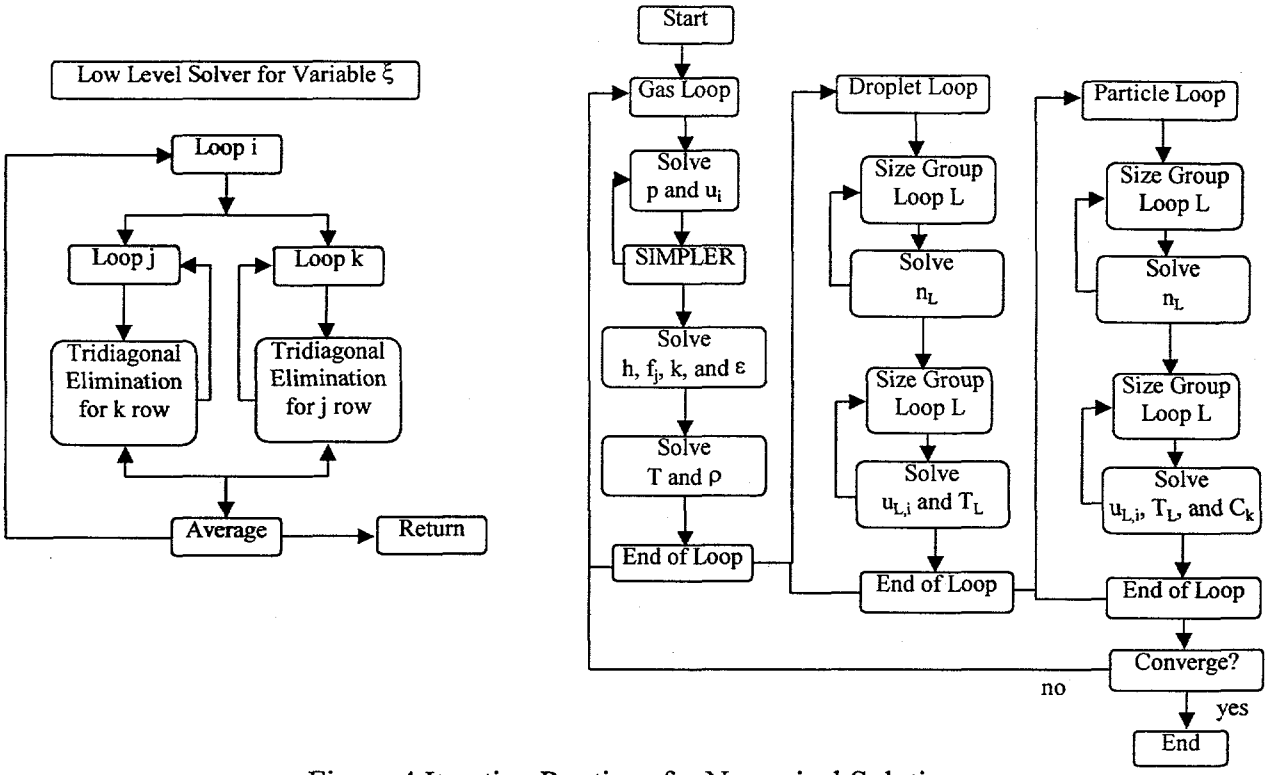


Figure 4 Iteration Routines for Numerical Solution

Numerical Convergence

A calculation is considered to have converged if the local and global mass balances of the three phases are smaller than a set of predetermined criteria, and the normalized residuals of the other differential equations are also sufficiently small. For an FCC flow calculation, convergence criteria defined by average mass residual (in dimensionless form, normalized by the gas mass flow rate) of all computational cells, are generally set at 10^{-10} for the gas phase and 10^{-7} for both the liquid and solid phases.

A grid sensitivity study needs to be conducted to select a grid system that gives independent numerical results regardless of further grid refinement in order to conserve computational time and still provide adequately accurate results. An important feature of the control volume approach is that it is conservative in terms of mass, energy, species, and all variables solved for via the transport equations, both locally and globally to a very high degree regardless of grid size. Generally in this application, ten to a hundred thousand nodes are used. A converged solution can be obtained in about 2000 iterations. Each iteration typically includes ten gas phase, three liquid, and three solid phase sub-iterations. On a Pentium™ III 600 personal

computer with 128 megabytes of random access memory, using a 32-bit FORTRAN compiler, this computation takes about four hours.

Exit Boundary Conditions

The question: "What is the implied boundary conditions at an outflow portion of the domain?" is a serious problem many face in CFD calculations. The free flow boundary condition often applies at the outflow exit. It has some success for calculation of a fully developed flow. In most practical applications, however, the flow is not fully developed at the exit, and the authors found that a fixed velocity gradient at the outflow exit yielded much better convergence. The exit velocity gradient can be determined by balancing global mass flow.

Numerical Instabilities and Debugging

Numerical instabilities are often encountered in a flow calculation. Some of them are due to programming errors; some are a consequence of the non-linearity of the equations; some are caused by singularities in the flow system, and some arise from using the finite precision computations of digital computers. For the programming errors, as long as they can be found, they are easy to correct. As for the other numerical problems, to find them is one thing and to resolve them is another. The resolution of these numerical problems usually requires the development of a new formulation and/or new numerical algorithms.

The authors found two very effective procedures to find and correct programming errors. One debugging procedure employs known flow symmetries that are a consequence of symmetric boundary conditions, it and includes the following steps: (1) run a full symmetric flow calculation, (2) compare the computed flow property numbers at corresponding symmetric locations, and (3) if the results are asymmetric, trace the computational steps back to the initial occurrence of the asymmetry and fix the problem. The other debugging procedure involves checking and maintaining very tight global mass and energy balances, and it includes the following steps: (1) check global mass and energy balances, and (2) if mass or energy does not balance, isolate the source of the imbalance and fix it.

Reaction and flow time scales are often different by one or more orders of magnitude. The difference of time scales can cause severe numerical stiffness problems. If the differential Arrhenius rate formulation is directly used in the source term of a lumped species equation during the flow field computation, a numerical calculation often diverges or continues unconverged indefinitely in a bounded oscillatory numerical instability.

Other numerical instability problems that the authors have encountered in various CFD applications are: (1) a flow reversal point in a dispersed phase (droplets or particles) of a multiphase flow where a velocity component changes sign, (2) a stagnation point in a dispersed phase where zero velocity is calculated, (3) high heat transfer rate between phases, (4) onset of droplet vaporization that drastically changes the heat balance in a computational cell, (5) the time scale difference between the flow of different phases, and (6) the difference between a continuous function used in the formulation and a discretized function used in the computation.

Code Validation

A multiphase and/or reacting flow CFD code carries a lot of flow physics and chemistry in it. But since it can only obtain an approximate numerical solution, verification and validation become an integral part of CFD application development. Verification involves comparison with analytical solutions and other numerical results. Validation involves comparison with

experimental data and data obtained from commercial systems when available. Validation is often difficult and never complete because of the limited availability and accuracy of the data. The availability of data for validation of real systems, such as FCC risers or pulverized coal combustors is often very limited for two primary reasons. First, it is very expensive to collect. Second, the very harsh environment in these systems can make data measurement extremely difficult if not impossible. Even optical methods may fail because the window may rapidly become covered with carbon or slag, etc.

CFD APPLICATIONS

Many CFD codes have been developed for various applications ranging from rocket engine combustion to microchip cooling. Some are developed in the universities and the national laboratories and some are available commercially. A CFD calculation can be used to: (1) provide detailed flow property information, (2) evaluate the impact of operating conditions on the performance of the system, (3) determine optimal operating conditions of the system, and (4) explore innovative concepts to improve the performance of a system. The following sections provide only a few examples of the CFD applications.

Fluid Catalytic Cracking Riser Reactors

In the past seven years, ANL has been working with the refining industry to develop computational capability for supporting advanced Fluid Catalytic Cracker (FCC) development, which could have a large impact on the public in general by lowering fuel costs and pollutant emissions [1,5]. As described earlier, a FCC-CFD code was developed specifically for the simulation of FCC riser flows involving three phases (gas, liquid, and solid) and many species reactions. A hybrid technique was developed to handle both hydrodynamics and complex chemical kinetics. A methodology was developed to extract many species cracking kinetic constants from a small set of measured yields under varied operating conditions. The code has been validated with several sets of test data from pilot- and commercial-scale FCC units. The code has been used to evaluate the impacts of operation/design parameters on the product yields of an FCC unit. The methodology and some CFD results will be described briefly in the following.

Extraction of Kinetic Rate Constants

There are thousands of oil product species produced in the cracking processes. The species can be lumped into smaller number of subspecies lumps for the analysis according to carbon numbers or boiling points. A subspecies is generated by the evaporation of oil droplets and/or the cracking reactions. Part of the subspecies is converted to lighter subspecies by the cracking reactions. An Ahrrenius type formula is used to express reaction rates of the cracking reactions. Kinetic rate constants including pre-exponential rate constants, activation energies, and orders of catalyst reactivity are affected by many factors, such as temperature, catalyst concentration, other local conditions in the reactor flow, etc.

A methodology has been developed to determine empirical kinetic constants for a particular riser, catalyst, and feed oil based on a relatively small number of experimental data sets for different riser operating conditions [14]. Using temperature as an example operating condition, the method includes the following steps: (1) select experimental test data sets for various temperatures, (2) establish the general trend of the temperature effect on the measured product yields, (3) setup the CFD code to compute product yields for the selected test conditions,

and (4) use iteration routines to adjust kinetic constants and activation energies to match predicted product yields with experimental data. Once a set of kinetic constants are determined, they are then used for the prediction of other test conditions and comparisons are made again between the predicted results and the experimental data for further validation of these constants. Chemical kinetic model constants determined in this way implicitly contain effects related to the local hydrodynamic flow field in a particular riser geometry and comparison between experimental yield results and results predicted using the extracted kinetic constant set in computations show very good agreement.

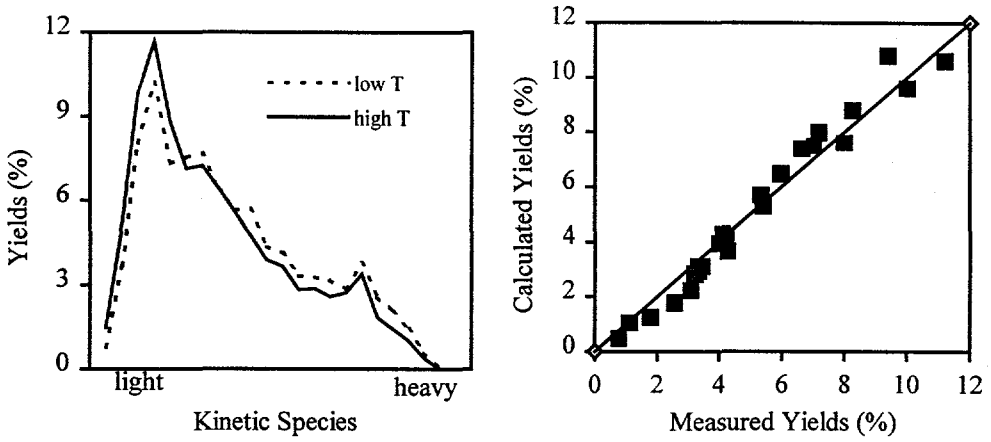


Figure 5 (a) Effect of Temperature; (b) Comparison of Calculated and Measured Data

Figure 5a shows the product yields of a FCC riser reactor for two cases of different temperatures. The product yields are used in the two iteration routines to determine a set of kinetic rate constants. Using the kinetic constants determined from the iteration routines, the CFD code was setup to do calculations for cases at temperatures other than the selected two. Figure 5b compares calculated product yields with the experimental data. The comparison shows excellent agreement.

Impact of Spray Injection Parameters on Gasoline Yields

The validated ICRKFLO code has been used for parametric studies to investigate the impact of operating and design conditions such as temperature, catalyst-to-oil ratio, feed injection conditions, and riser configuration. The following presents some results of parametric studies of feed injection condition effects.

In FCC refining systems, nearly all the gas phase mass flow comes from vaporizing feed oil sprayed into the FCC riser and all the heat for vaporization as well as the endothermic cracking reactions comes from hot regenerated catalyst particles. Therefore, the refining process is very much driven by phase interactions, which is strongly dependent on the feed injection conditions. In simulation studies the spray injection parameters that are easy to isolate and vary while holding other conditions constant are the mean droplet size, the mean spray injection velocity, and the spray injection angle. These conditions may not be independent of each other in the operation of actual spray nozzles in a commercial scale FCC unit. They are used in CFD parametric studies, however, because they do provide both clear and physically reasonable insights into the impact of these parameters on spray penetration, spray vaporization rates, and petroleum cracking yields. Such insights into very complex interacting multiphase phenomena

can provide a basis for improving performance through better nozzle design, which may be verified by laboratory testing of the nozzles alone, as opposed to testing an entire FCC reactor with various nozzle designs installed.

A number of simulations were performed with varied spray injection conditions for one pilot scale riser and two different commercial risers. It was found that two injection parameters, i.e., droplet size and injection velocity, had a significant impact on the product yields. Furthermore, a functional correlation was found between the calculated product yields and a combined injection parameter. The combined parameter is defined as the injection Reynolds number as shown in Equation (6).

$$Re_{inj} = \frac{2\rho_\ell r_k V_{inj}}{\mu_\ell} \qquad (6)$$

in which ρ and μ are oil vapor density and viscosity, respectively, r_k is the mass mean droplet radius, and V_{inj} is the feed oil injection velocity. The injection Reynolds number represents the ratio of injection inertia forces from droplet momentum and droplet drag forces.

Figure 6a shows calculated gasoline yields versus injection Reynolds number. It indicates that all the data can correlate in a smooth function and there is an optimum Re_{inj} number that produces maximum gasoline yields. Figure 6b and 6c display the droplet number density and gasoline concentration distributions for the conditions of low, optimum and high Re_{inj} numbers. Clearly, at very low Re_{inj} number, droplets do not penetrate well due to small inertia and at very high Re_{inj} number, the evaporation of droplets occur slowly due to large injection inertia. At the optimum Re_{inj} number, droplets penetrate the flow to yield excellent catalyst/droplet mixing and evaporate quickly enough for high degree of cracking. This suggests that a maximum gasoline yields can be produced by adjusting the spray injection conditions.

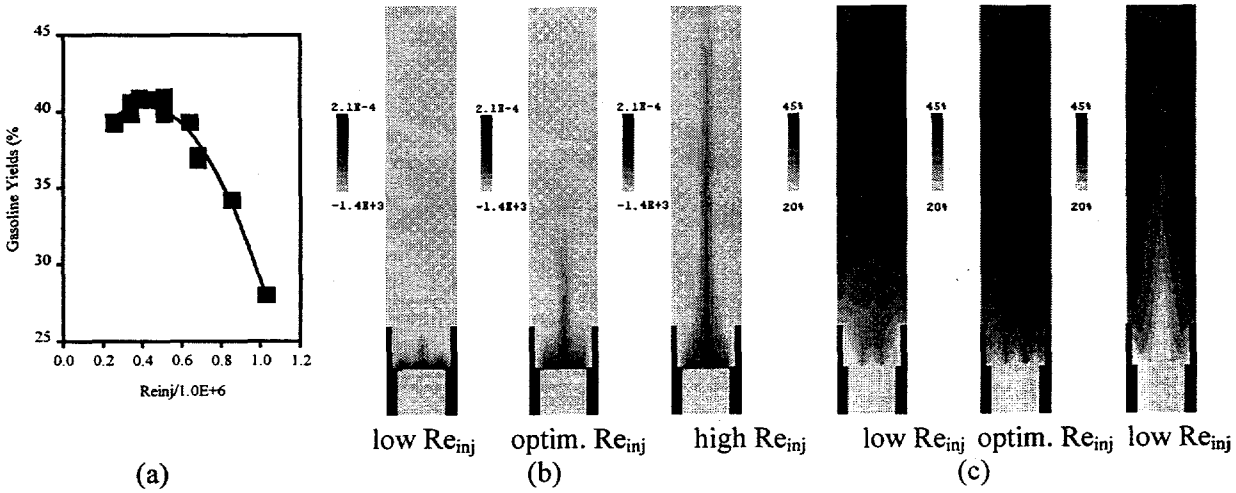
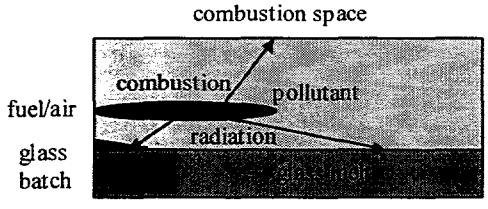


Figure 6 (a) Gasoline vs. Injection Renolds Number; (b)Droplet Number Density Distributions; (c) Gasoline Concentration Distribution

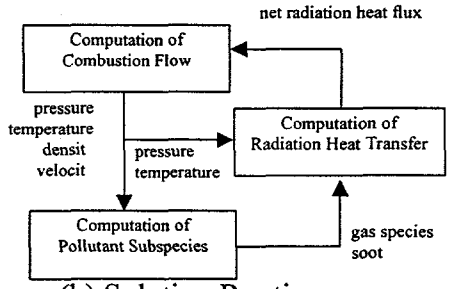
Glass Furnace

Glass furnaces are one of the principal users of natural gas in the U.S., consuming about 5 billion cubic meters per year, and they emit a significant amount of NO_x. Approximately ¾ of the energy from natural gas in these furnaces is used for melting and most of these furnaces consume about twice the theoretical amount of natural gas needed to melt the glass. CFD simulations are used to investigate the flow characteristics in the glass furnace so the energy consumption and pollutant emissions can be reduced, and glass quality can be improved. A sketch of a glass furnace is shown in Figure 7a. Fuel and oxidizer are injected into the furnace for burning. The heat of combustion is used to melt the sand and cullets and produce glass products.

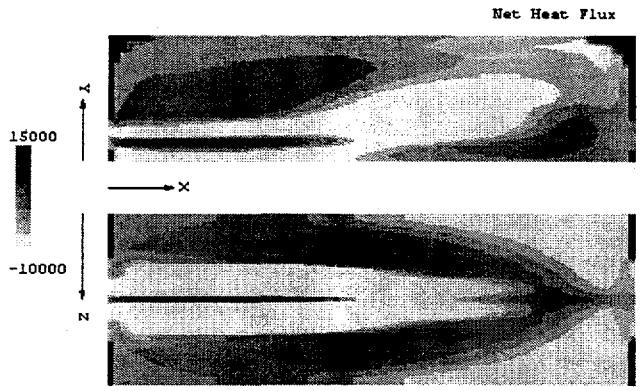
A CFD code, ICOMFLO, was used to simulate the combustion space of the glass furnace and determine the heat transfer and NO_x emission from the combustion space. Because of the high temperature environment in the furnace, radiation becomes the dominant heat transfer mode. ICOMFLO uses a three step de-coupled computational scheme and divides the combustion species into two groups: major species and subspecies. The three step scheme includes the computations of (1) combustion hydrodynamics, (2) formation and transport of pollutants, and (3) radiation heat transfer. The three computational steps are linked together through an iteration routine as shown in Figure 7b. The code first computes the major flow properties of the combustion flow in the furnace by assuming a uniform radiation heat flux in the space. In this step, pressure, temperature, density, velocity, and species concentrations are locally computed. A combustion model of the major species is needed in this step to establish an initial temperature field. Next, a kinetic model of the subspecies is used to calculate the formation and transport of the subspecies based on the major flow properties computed in the first step. Then, a radiation heat transfer model is used to calculate local net radiation heat flux (the balance of emission and absorption) based on the temperature and pressure calculated in the first step and the species concentrations calculated in the second step. The radiation participating media in a glass furnace include carbon dioxide, water vapor, and soot in the combustion space and glass in the glass melt flow. Since radiative emission and absorption of these media depend strongly on wavelength of the radiation, a spectral radiation heat transfer model is used. The code can be used to calculate both the heat transfer rate (see Fig. 7c) and the NO_x concentration in the combustion space of the glass furnace.



(a) Sketch of the Glass Furnace



(b) Solution Routines



(c) Net Heat Flux in the Furnace (side and top views)
Figure 7 Simulation of a Glass Furnace

Magnetohydrodynamic Power Generation System

Magnetohydrodynamic (MHD) power generation deals with an electrically conducting flow in the presence of a magnetic field. It has attracted much interest from utility industries because it can in theory attain higher overall efficiency and produce less pollutants compared to a conventional coal-fired power plant. The U.S. Department of Energy sponsored a proof-of-concept program with the goal of commercialization of MHD power generation in the 1980s. Figure 8 shows a conceptual sketch of a typical MHD system. The system consists of five major components: a first stage swirl combustion, a de-swirl section, a second stage combustor, an MHD channel, and a diffuser.

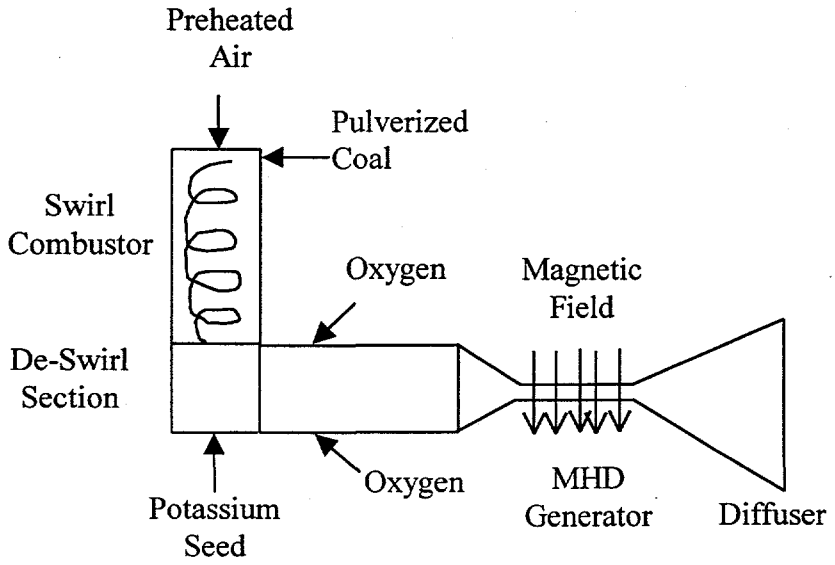


Figure 8 Sketch of an MHD Power Generation System

Among the most important considerations for the program are the attainment of high temperature from the two-stage combustion and the injection of a seed material, i.e., potassium, to achieve the desired electric conductivity in the gas flow and produce electric power. For the POC program, TRW built a 50 MWt two-stage pulverized coal combustor. The first stage

combustor was a common swirl combustor and the second stage combustor was a new design. The performance of the second stage combustor depends heavily on completing combustion with minimum heat loss and mixing to achieve a uniform dispersion of the seed vapor. The distortion of gas temperature and seed vapor profiles caused by poor mixing, may significantly lower the electric conductivity and subsequently degrade the MHD channel performance. ANL used several computer codes to simulate the entire MHD system. A CFD combustion code was used to investigate the flow characteristics in the second stage combustor [15]. The computational results showed that the injection angle and velocity have a strong impact on the combustion efficiency and temperature uniformity. Furthermore, an optimal injection angle of approximately 130 degrees for maximal power generation was determined. Later, the experimental of the testing facility confirmed the numerical prediction of the optimum oxygen injection angle.

Pneumatic Transport Pipelines

A pipeline was designed to transport pulverized coal with nitrogen from storage bin to blast furnace. The long pipeline consisted of many elbows. Severe operating problems were encountered. The problems could be related to particle pile-up in elbows. A CFD code was used to investigate these problems [16].

Gas-solid interactions are the dominant processes in such a flow system. ANL has developed a CFD code with a new and improved model to treat the gas-solid interactions. The code was validated previously with the experimental data characterizing particle number density distributions in gas/particle pipe flows. For this investigation, an additional validation was conducted. The pressure drops along the pipeline were measured. The pressure measurements were compared with the results from the CFD calculation. The comparison showed good agreement between calculated and measured pressures. Once validated, the code was used to investigate the particle pile-up problems. The analysis of the gas-solid flow in elbows revealed that the elbows most likely to experience pile-up problems were those elbows receiving input from a horizontal pipe and then passing the flow into a vertical pipe. Decreased particle mass flow rate or decreased average particle size could decrease the likelihood of particle pile up.

Ramjet Engine Combustion

In the late 1980s and early 1990s, a conceptual hypersonic ramjet aircraft was under development. The developers of the conceptual aircraft were considering using a wind tunnel test facility on the ground to measure the performance of the ramjet engine in order to avoid the difficulties associated with obtaining high altitude, in-flight measurements. An arc heater was used in the ground test facility to heat up a hydrogen flow before it entered the combustion chamber of the ramjet engine. In the heating process, the copper electrode of the arc heater was eroded by vaporization and copper vapor contaminates entered the combustion flow. A critical question, related to the viability of the ground test facility, was whether the copper contaminants affect the performance of the hydrogen-air combustion.

ANL conducted an extensive literature survey and found that copper (either vapor or solid particles) is an effective catalytic agent in the hydrogen combustion reactions [17]. The copper can speed up the recombination rate of the hydrogen atoms. A kinetic model was developed for the copper-hydrogen interactions. The kinetic model was incorporated into a CFD code for the simulation of the ramjet combustion flow. CFD calculations were made with the copper contamination and without contamination. The computed combustion rates and flame

lengths showed significant differences between the two cases. This result suggested that the flow measurements in a ground test facility could be much different from those actually measured in-flight. Since the in-flight measurements are much more expensive and difficult to obtain than the ground measurements, the CFD code can be used to interpret the ground test data and convert the data to the in-flight results.

Gas Turbine System

A gas turbine engine combustor increases the enthalpy of the working fluid by combustion and produces temperature distributions acceptable to the turbine by the subsequent dilution of resulting products with additional air. Some operating conditions, such as ignition, acceleration, idle, etc., are apparently transient in nature with a non-uniform distribution of flow variables on transversal section. During system operation, physical processes in individual components of a gas turbine system are strongly coupled. Influences between connected components, such as diffuser and liner are important to gas turbine performance. A CFD calculation for a complete annular combustor - from the compressor exit to turbine inlet - is needed for investigation of the interaction between the diffuser and the combustor.

In recent years, numerical methods have been developed for the simulation of gas turbine combustor flows [18,19]. For a long time, diffuser and liner were simulated separately due to the limitation of the capacity of computers. Recently, a numerical simulation of combustor-diffuser flow interactions using the KIVA-3V code was conducted [20]. KIVA, a transient, three-dimensional, multiphase, multicomponent code for the analysis of chemically reacting flows with sprays was developed at the Los Alamos National Laboratory [21]. The code uses an Arbitrary Lagrangian Eulerian (ALE) methodology on a staggered grid, and discretizes space using the finite-volume technique. The code uses implicit time-advancement with the exception of the advective terms that are cast in an explicit but second-order monotonicity-preserving formulation. Arbitrary numbers of species and chemical reactions are allowed. A stochastic particle method (Lagrangian approach) is used to calculate vaporizing liquid sprays, including the effects of droplet collisions and aerodynamic breakups. Although specifically designed for performing internal combustion engine calculations, the modularity of the code allows for easy modifications to allow it to be applied to a variety of hydrodynamics problems involving chemical reactions.

In the simulation of gas turbine combustors, the KIVA code was modified to set up proper boundary conditions. A typical annular combustor including a diffuser, outer and inner annuli and a liner was employed. Computations were conducted in a section of the combustor of 22.5° from the inlet of the diffuser to the exit of the liner. Jet-A was used as the fuel. Several validations were made by comparing computational data with experimental data and semi-empirical data. Static pressure recovery coefficients along the inner and outer walls of the prediffuser and combustor casing were obtained and agreed well with the measurements. Combustion efficiency and overall temperature distribution were predicted in reasonable agreement with those from a semi-empirical approach. Effects of non-uniform profiles of velocities at the inlet of the diffuser on combustion performance were investigated. Computations were also performed to study the effects of spray inlet conditions on the combustion performance, and NO_x emissions studies were also conducted. All the results showed reasonable trends and provided a foundation for further study of the transient behavior of flows in a compressor-combustor system [20].

Fluidized Bed Combustors

Fluidized bed combustion technology attracts intense commercial interest for its capability of burning high-sulfur coal in a more economic and environmentally acceptable manner, despite the unsolved erosion problem. Detailed knowledge of the complex phenomena of solids circulation and bubble motion in the bed could enhance the understanding of the erosion problem and find solutions. ANL has developed a two step methodology [22] to investigate local erosion phenomenon in bubbling fluidized bed combustor (FBC) systems: (1) use a state-of-the-art two-phase two-dimensional hydrodynamic computer model (FLUFIX) to compute temporal and spatial distributions of the flow properties in an FBC and (2) use spectral analysis and several separated erosion models to evaluate flow dynamics and local erosion patterns and rates. The spectral analysis uses the computational hydrodynamic results of a two-dimensional generic fewtube FBC system to correlate flow properties, porosity, pressure and velocities, as well as to determine oscillation modes and bubble propagation speeds. The findings from this analysis include: flow properties have major oscillation modes of frequencies ranging from 0.7 to 4 Hz; porosity and pressure oscillations propagate from the bottom of the bed up with propagation speeds ranging from 0.4 to 1 m/s; and pressure is well correlated with the lagging porosity at a location [23].

SUMMARY

The rapid advancement of computational capability including speed and memory size has prompted the wide use of computational fluid dynamics (CFD) codes to simulate complex flow systems including industrial multiphase and reacting flow. A CFD code can be developed with the based on flow dynamics and related physics and chemical kinetics, numerical techniques, and computer science. The governing equations are derived from the fundamental conservation laws of mass, momentum, and energy. Various numerical methods are currently available to convert the governing differential equations to algebraic equations and iterative routines have been developed to find approximate solution for the algebraic equations. Many phenomenological models needed for the simulation of complex processes in a practical energy system, like turbulent diffusion and turbulent phase interactions, combustion kinetics, interfacial interactions, radiation heat transfer, etc. have been developed. With verifications and validations, CFD simulations can be used to evaluate practical energy systems. These simulations can: (1) provide detailed flow property information, (2) evaluate the impact of operating conditions on the performance of the system, (3) determine optimal operating conditions of the system, and (4) explore innovative concepts to improve the performance of a system. Experience with many applications indicates that the use of CFD simulation can help reduce energy consumption, pollutant emissions, and improve the quality of the products.

Acknowledgments

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