The Fluidity of Thought and Vision: 40 Years of CFD at Iowa State

Present at the birth of computational fluid dynamics, lowa State researchers continue to push back the frontiers of this lesser-known but vital engineering discipline.





TUDYING GENERAL FLUID MECHANICS AND HEAT TRANSFER AS A GRADUATE STUDENT IN THE 1960S, MECHANICAL ENGINEERING PROFESSOR RICHARD H. PLETCHER HAD LIMITED EXPOSURE TO THE ANALYTICAL AND EVEN LESS TO COMPUTATION. BUT THOUGH HE COULD SOLVE CERTAIN FLUID MECHANICS EQUATIONS BY RUNNING REAMS OF PUNCHED CARDS THROUGH THE SCHOOL COMPUTER, HE FOUND LITTLE SUPPORT FOR THAT APPROACH IN THE PRECINCTS OF ACADEMIA.

"My adviser tried to give me some advice," Pletcher remembers, "which was 'don't mess with computational things; the future would be in experiments'—he thought the computer business was a diversion that wouldn't be very profitable."

Undeterred, Pletcher signed on with United Aircraft (today United Technologies), where he developed algorithms for solving flow problems. This in turn became the basis for a paper on numerical methods for early CFD applications he would submit for publication shortly after coming to Iowa State in 1967.

One of the lesser-known engineering disciplines, today computational fluid dynamics is critical across several areas, from the modeling of airflows over jets to the design of multimillion-dollar reactors for pharmaceuticals. The ability to predict the movement of liquids, gases, and solids, whether singly or in multiphase systems, has allowed innovation in numerous industries to pace and parallel the everaccelerating power of computation.

Yet given the relative scarcity of computing resources in the 1960s—even in academic settings the injunction of Pletcher's adviser was perhaps not as outlandish then as it may sound to modern ears.

Crossing disciplinary boundaries

Nonetheless, although initially hired to teach courses in fluid mechanics, Pletcher continued to dabble in computation, hauling stacks of punched cards to Iowa State's mainframe. Using the computer, he would solve the boundary-layer equations, a reduced set of the Navier-Stokes equations modeling viscous flow over solid surfaces.

"We'd estimate the friction exerted on a wing or any solid body, and I'd also include heat transfer," Pletcher recalls. "I'd solve the energy equation that would determine if the surface was hotter or cooler than the air, and we'd estimate the transfer of energy."

Before long those methods paid off in Pletcher's classroom, so Pletcher paid a visit to the Department





Above: Detail of a key punch machine typically used to enter CFD data into an institutional mainframe. **Below:** About 10,000 punched cards would be needed to enter enough data to represent the computer code that produced this image.



An impinging-jets microreactor for microscale particle-image velocimetry ("microPIV") experiments.

FOX, NIRT RESEARCHERS PAVE WAY FOR NEW CFD CODES

IN 2004 RODNEY FOX HEADED UP A NANOSCALE INTERDISCIPLINARY RESEARCH TEAM COMPRISED OF RESEARCH TALENT FROM IOWA STATE, KANSAS STATE UNIVERSITY, AND THE UNIVERSITY OF MINNESOTA. SPONSORED BY THE NATIONAL SCIENCE FOUNDATION, THE OBJECT OF THE MILLION-DOLLAR EFFORT, NOW IN ITS FINAL YEAR, IS TO BETTER UNDERSTAND THE KINETICS OF PARTICLES AT THE NANOSCALE LEVEL SO THAT THEIR AGGREGATION MIGHT BE BETTER CONTROLLED. THE INFORMATION GATHERED BY THE SCIENTISTS MAY ULTIMATELY FIND ITS WAY INTO NEW CFD CODES.

Controlling aggregation at the nanoscale, Fox says, will affect a host of applications, including systems for delivering drugs across tissue barriers too complex to be penetrated by the microparticles used in other systems. New composite materials having both a matrix phase and a nanoscale phase would exhibit greatly improved strength-to-weight ratios, allowing for enhanced fuel efficiency in aircraft and vehicles. Even simple commodities such as paints that have both a fluid phase and a particulate phase would be improved, resulting in products with greater longevity and uniformity.

"If we can understand what happens, then we can control it," says Fox. "Right now this is done empirically—and that's kind of a hit-and-miss proposition." The research team is examining the behavior of particles at various stages of the chemical reaction process within their own areas of expertise, including quantum mechanical codes, particle surface chemistry, molecular dynamic simulations, and large-scale clusters. "It's a sort of multi-scale problem," Fox adds, "and that makes it interesting—and difficult."

of Aerospace Engineering and Engineering Mechanics. There he met Dale Anderson and John Tannehill, who themselves had begun to investigate the use of numerical methods to model airflows over surfaces.

The three decided to develop electives to be offered across their respective departments, determining that the courses should be team taught—the field was so undeveloped that no one had sufficient knowledge to cover the subject on his own. Their complementary interests would result in one of the seminal textbooks in the emerging discipline. First published in 1984, by 1997 *Computational Fluid Mechanics and Heat Transfer* had gone into a second edition as well as translation into Russian.

Another factor driving the early development of CFD at Iowa State was the relationship Pletcher and his colleagues enjoyed with U.S. government labs, especially NASA Ames in California. In fact, Pletcher notes, a number of the branch and division chiefs at NASA Ames were Iowa State graduates, a connection that enabled Iowa State faculty and students to work remotely off NASA mainframes. By 1980, that connection resulted in major grants from NASA to Iowa State and a handful of other U.S. academic institutions to develop advanced CFD programs.

"That was a huge step that we got recognized as one of the top five programs," Pletcher says. "Iowa State would stand up with some very prestigious schools in the field."

ChemE 'reacts' to new discipline

Yet while Pletcher and his colleagues were building a curriculum directed largely toward aerospace and mechanical engineers, the 1980s would witness the advent of the personal computer and the emergence of chemical reaction engineering as the latest discipline to be revolutionized by CFD.

As an undergraduate roaming the Kansas State campus with an armload of punched cards, Herbert L. Stiles Professor of Chemical Engineering Rodney Fox was ready for the revolution. For if computational fluid dynamics was in its infancy for aerospace engineers in the 1970s, it was not even a gleam in the eye of scientists such as Fox, an internationally recognized authority in the use of CFD for chemical reaction engineering.

"We had a big computer you would stick the cards in," Fox remembers. "You had to write a program and



jump through hoops, and in the end you could just get digits to come out instead of a graph."

More than aesthetics, the challenges facing Fox and other chemical reaction engineers have spurred them to employ some of the same methods as their mechanical and aerospace counterparts. However, Fox notes, chemical engineers were not so much concerned with grids, algorithms, and other numerical methods as with the kind of modeling that would illuminate the physics inside of reactors.

"We were trying to figure out how fluid mechanics affect chemical reactions," Fox says. "We were using overall models that didn't tell us what the velocity field was, so we had to try something different."

Before CFD, Fox notes, engineers would typically build a small model reactor in the lab, test it, and, based on the results, move to a pilot-scale reactor. If the pilot-scale reactor performed well, then work could proceed on a large-scale commercial reactor.

Yet as you scale up, Fox observes, temperatures tend not to remain uniform due to heat transfer along the boundaries of the reactor. And so where a chemist might get 90% usable product from the outlet of a lab-scale reactor, that might drop to 50% at the pilot scale and even less in a full-scale reactor, barring total redesign of the system.

"Then you have to figure out what you did wrong," Fox adds. "It's all done empirically: you have rules, but you don't have any way to know what's going on inside. You just have to figure out how you would change the design from one scale to another."

And that could be costly: while lab-scale reactors might run tens of thousands of dollars, pilot reactors could cost a million to build, and full-scale commercial

"Calculations are cheap—you don't have to build something that costs \$100 million."

reactors up to \$100 million or more. By more effectively modeling chemical reactions *before* scaleup, engineers could save clients considerable time and money.

"It's a kind of acceleration to get more efficient processes," Fox says. "Calculations are cheap—you don't have to build something that costs \$100 million."





Aerospace engineer Z. J. Wang among the > collection of antique aircraft components

> But that's not to say those calculations are simple. As computational capacity has expanded, chemical engineers have added increasing detail to simulations, examining the complex physics of chemical reactions in addition to the turbulent flows that most concern aerospace and mechanical engineers.

> As Fox notes, chemical engineers are not interested so much in the velocities of flows as in how velocity

"Now with the CFD code, you break the reactor, say, into a million cells...

> affects heat and mass transfer in chemical reactions. And when you factor those into the simulation, you increase exponentially the amount of information that must be processed to achieve a reliable model of a chemical reactor.

> "In our old reactors," Fox observes, "we essentially treated our models as one big cell. Now with the CFD code, you break the reactor into, say, a million cellsand then model what goes on inside each of those boxes."

This incredible articulation of detail was driven not just by expanded computational capacity, but also by the demands of the commodity chemical industry. By the 1980s engineers were increasingly unable simply to guess at the internal processes of scaled-up reactors, but instead required more detail to accurately predict reactions. This gave rise to the first commercial CFD codes for the industry by the mid-1980s, as well as to the first experts in applying CFD to reaction engineering.

One of those experts, Fox is careful not to oversell the power of CFD for chemical engineering. The codes, he notes, are just numbers, and it remains for the engineer to plot surface velocities and the locations of concentrations, among other factors. And while it may no longer take a month to finish a calculation, speed takes a back seat to expanded capacity.

"The geometry's complicated," Fox says, "so we spend less time trying to make the code faster and more trying to put more chemistry into it. That way, we can predict real chemistry instead of some simple 'A+B' thing."

Modeling at the nanoscale

26 INNOVATE > FALL 2007 IOWA STATE UNIVERSITY COLLEGE OF ENGINEERING Yet for all of its predictive power, CFD offers only a





a) CFD image of the scattering of acoustic waves by two cylinders, computed using the spectral volume method. b) (from top) Original geometry, computational surface mesh, and computed thermal map on the surface of an engine. c) Iso-surfaces of downwash generated by hovering helicopter rotors. d) Computational mesh and contours of vorticity magnitude for a generic supersonic missile.

simulation of an infinitely complex chemical reaction that cannot possibly account for everything that happens inside a given reaction chamber.

Most of the equations upon which a simulation is based, Fox notes, are what are known as "initial value problems" that show a fixed reaction field and then that same field at another point in time. The difference between any two points represents "shear," which impacts reacting flow at all points of the simulation. To the extent these are accurately rendered across the entire simulation grid, the CFD engineer can more or less accurately determine what a given point or cell will look like at a given point in time.

"Then you go to every box and figure out what moves through in the next time instant," Fox says. "And you do that over and over."

If your simulation is accurate, he adds, the resulting model will, ideally, represent exactly what the fluid is doing. But engineers work not in the ideal but the real world, with all its constraints and ambiguities. Besides, Fox notes, that comprehensive ideal would generate too much data for engineering purposes. So the engineer instead settles for the average values generated from a series of such "snapshots." Still, Fox stresses, it is not the size of the reactor that concerns chemical engineers so much as the speed of the reaction relative to mixing time, a challenge that can impact the design of scaled-down micro-reactors as much as those \$100-million behemoths.

Recently, Fox has been involved with two projects sponsored by the National Science Foundation's Nanoscale Interdisciplinary Research Team (NIRT) program. In one, a team of Iowa State chemical engineers has joined colleagues from other departments and universities to develop strategies to prevent nanoparticles from aggregating into larger units that might alter their fundamental properties, a project of special interest to the pharmaceutical industry.

Another NIRT to which Fox lends his expertise involves micro-reactors to engineer particles of a specific size for medical applications. By mixing chemicals in such small reactors, Fox says, CFD codes can better simulate reactions by eliminating variables such as turbulence. And better codes mean tighter control of what that reactor ultimately produces.

"The pharmaceutical industry might want particles that are only 100 nanometers, because that's the only size that can go into the bloodstream," Fox observes. "React it one way, they might all aggregate into big globs; do it another way, you get individual particles in which you can control the size. So we spend most of our time looking at models that go into CFD codes to predict things like particle size distributions and chemical distributions, not just fluid mechanics."

An aid to the imagination

"It could take another 50 to 100 years...to solve such turbulence directly for flight configurations."

> Still, the seemingly greater demands of CFD in chemical reactions in no way diminish the horizons of CFD in traditional aerodynamics, which still represents the majority of applications in the field. Even Fox concedes this dominant position, citing the Boeing Corporation's unveiling this year of its groundbreaking 787 "Dreamliner," a carbon-fiber miracle of structural toughness and fuel efficiency designed using the company's CFD proprietary codes without the use of wind tunnels.

> If Dick Pletcher embodies the birth of CFD, then aerospace engineer Z. J. Wang represents its future. Born at the dawn of the space race, Wang's childhood fascination with rockets and airplanes led him first to China's National University of Defense Technology, where he won the opportunity to do doctoral work in the United Kingdom at the University of Glasgow, followed by a postdoc at Oxford.

> Wang spent the 1990s in private industry at Alabama's CFD Research Corporation where he developed several highly successful commercial codes, including CFD-FASTRAN, widely used for studying external aerodynamics and acoustic instability inside the combustion chambers of rockets. He left in 2000 to start his academic career at Michigan State and came to Iowa State in 2004 to take advantage of the university's profile in the field.

> Like Fox, Wang points to Boeing and other manufacturers who favor CFD codes that can simulate conditions impossible to replicate in wind tunnels. "Take hypersonic flow," he says, citing one of his own specialties. "It may not be possible to make wind tunnels generate conditions such as Mach 25. For CFD, that's just another input parameter."

> Yet for all its power, Wang concedes, CFD essentially articulates quantitatively what the human mind is capable of in a qualitative sense. In that regard, CFD serves as the perfect aid and complement to

the imagination. And as computation becomes more powerful, minds such as Wang's envision greater challenges for the field.

One such challenge is turbulent flow, a problem far more intractable than the relatively simpler issues associated with laminar flow vectors. But while inefficiencies caused by the inability to account for turbulence when modeling a chemical reaction might cost money, in aerodynamic design they can cost lives, as with wind shear in the landing and taking off of aircraft.

"Wind shear involves a lot of small-scale vortices going through the flow field," Wang notes, "and CFD currently has problems with unstable vortices. It could take another 50 to 100 years of computer development to solve such turbulence directly for flight configurations."

The turbulent vortices of man-made shear are nearly as resistant to computational analysis as atmospheric wind shear. Still, working on a project funded by the Defense Advanced Research Projects Agency, Wang seeks to develop software that could redesign helicopter blades to reduce their noise signature as much as 90%—a boon to soldiers working in environments such as Iraq and Afghanistan, where approaching helicopters can give guerilla forces advance warning of attacks.

'A romance with computers'

As challenging as that may be, the CFD-powered flights of fancy Wang takes these days soar far beyond noise reduction. Over the next decades, he sees flight modeled even more closely after nature itself. Insects, birds, even fish—all are subjects for analysis as computation increasingly achieves the power to represent nature's most detailed dynamics and infinitely more efficient economies of motion.

And he sees codes that model activity at the cellular level, as the leap in computation and visualization that brought Fox and other chemical engineers into the field yesterday is matched by technologies capable of bringing the power of CFD to bear on micro- and even nano-levels of detail tomorrow.

That's a vision shared by Fox at mid-career. And as his own career winds down, Pletcher himself is no less fascinated by the field's future than by the excitement of those earlier, pioneering years in CFD.

"It's been quite a romance with computers," Pletcher muses. "I feel lucky I was able to get in, maybe not at the beginning, but in some of the early stages where we could make some advances. It was a unique time."