My Life and Career (So Far) in Combustion Chemistry

That is a pretty pretentious title, but I promised that I would write something autobiographical in this space, and I will do that. However, first I want to thank everyone who contributed to the Festschrift. When Stephen Klippenstein told me that he and Craig Taatjes had gotten approval for it (against my advice), I envisioned a situation where the issue had only two papers, both co-authored by Stephen. Luckily that turned out not to be the case. At the time of this writing there are forty-three manuscripts at various stages of review. I am extremely grateful to Craig and Stephen, to the editors of the journal, and to all the authors for the tribute. It is far and away the most flattering thing that anyone has ever done for me in my career.

I am the ultimate baby boomer: I was born in Huntington, West Virginia, in 1946, roughly nine months after my father returned home from the war. Of course, baby boomers are also the "children of the sixties"; I entered high school in 1961 and graduated from college in 1969. Membership in these two groups has affected how I think about almost everything. My mother's family has lived in Virginia and West Virginia as far back as anybody knows. However, my paternal grandfather was born in Blackpool, England. He joined the merchant marine and met and married my grandmother in Halifax, Nova Scotia, where my father was born, the second of what was ultimately to be four children.

Very soon after my father was born in 1913, the family moved to West Virginia, where my grandfather worked in the coal mines. He became a union organizer for the United Mine Workers, which caused the family great hardship. He would get a job; then the company would find out what he was doing and fire him. Thus, the family moved from camp to camp until my grandfather could no longer find work. My father remembered one instance vividly. Around Christmas time, with snow on the ground, my father returned home from school only to find the family furniture in the front yard, where the company thugs had put it. My grandfather was forced to find shelter for his family without notice. In those days, the company owned everything—the mine, the housing, and even the "company store." Ultimately, my father was forced to quit school, at age sixteen, and go to work in the mines to help support the family.

My father worked in the coal mines for twelve years, during which time he met and married my mother. My mother was the youngest by far of eleven children (she had several nieces and nephews who were older than she was). My parents had been married for only a couple of years when World War II broke out and my father enlisted in the navy. He served in the Pacific until the end of the war.

I am an only child. I would now characterize our family when I was growing up as lower middle class, with my father holding two or three different jobs, none of them in the coal mines, however. Unlike most of those honored with Festschrifts, I did not particularly like science as a youngster. Although I always had a gift for mathematics, it was not until I took chemistry and physics in high school that science began to appeal to me. Instead, I fell in love with sports, particularly baseball and basketball, at about age eight. Pretty much every night in the spring, summer, and even early fall, my father and I would play catch. There was a period of years when I could name every player on every major league baseball team, tell you what position he played, where he hit in the batting order, and what his batting average was on any given day (along with any other pertinent statistics). Until I graduated from high school my father and I routinely made three trips a year to Cincinnati, Ohio, to see the Reds play, mostly for Sunday double-headers. I will never forget the first major league baseball game I ever saw, between the Reds and the Brooklyn Dodgers, in June of 1955. In the first game of the double-header a Cincinnati pitcher named Johnny Klippstein had a no-hitter going until there was one out in the ninth inning. Then Jim Gilliam got a bloop single over the second baseman's head, leaving Klippstein with a one-hitter. As a basketball player, I simply lacked talent. Even though I could shoot the lights out, I was too short to play forward and too slow to play guard. My hand-eye coordination stood me in better stead in baseball, which I played through high school, having most of my success as a pitcher.

It was never a foregone conclusion that I would go to college. As far as I know, nobody on either side of my family had ever gone to college before. However, I was a good student (ultimately high school valedictorian), so my parents agreed that I should go to college, although my mother wanted me to stay close to home. Because of my ability in mathematics and science, and to maximize potential job opportunities when I graduated, we decided that I would major in engineering. I had been fascinated by the space race since the launch of the first Sputnik in 1957, so I decided to go into aeronautical (aerospace) engineering.

I applied to several colleges. Even though MIT offered me a fairly generous financial aid package, including scholarship and loans, I chose to go to the University of Cincinnati. This choice had several advantages. It was close to home (which pleased my mother), had a good engineering college, and its engineering co-op program, together with a merit scholarship, offered the opportunity of getting a degree at minimal cost. With the co-op program, it took five years to get a bachelors degree. My co-op job taught me one thing: working as a bachelor's degree engineer is not very stimulating. Ultimately, this recognition was probably behind my choice to go on to graduate school. However, my job did introduce me to the San Francisco Bay Area; I fell in love with San Francisco the first time I ever saw it. The city and the area have always seemed like they should be my home.

In college, the classes I liked best were in mathematics and physics, not so much the engineering courses. All my technical electives were mathematics classes, and the class that left the most lasting impression on me was one in modern physics, where I learned for the first time about quantum mechanics and relativity.

After graduating from Cincinnati, I went on to graduate school at Cornell, again in aerospace engineering. I chose Cornell over a number of other options (including MIT, Princeton, and Stanford), because the department was small and seemed more like an applied physics department than one in engineering. The course list included things like plasma physics, magnetohydrodynamics, advanced kinetic theory of gases, and rarefied gas dynamics. There were strong research efforts in these areas and in the traditional areas of fluid mechanics and aerodynamics, as well as work related to chemical and gas dynamic lasers. Cornell has a simple organizational device that I think is very effective in promoting interdepartmental cooperation. Cornell

10.1021/jp079504a CCC: $37.00
Published on Web 05/10/2007

distinguishes between "departments" and "fields". A professor may be employed by one department to teach classes, etc., but he may be a member not only of that "field" but others as well. This means that he can supervise graduate students who nominally are students in other departments. This simple device fosters a spirit of cooperation among departments that I have not seen at other schools, and I benefited greatly from it. I took classes not only in the aero department, but almost as many in the chemistry and physics departments. This provided me with extremely important background for my future research career. Ultimately, my thesis research was supervised by Simon Bauer from the chemistry department, in cooperation with Tobe de Boer and Ed Resler from the aero school; notably Terry Cool served as my minor advisor in applied physics.

I enjoyed my time at Cornell. I met and married my wife, Connie, while we were both students there. There is one final Cornell experience that made a lasting impression on me—I took statistical mechanics from Ben Widom. His lectures invariably started on time and ended on time. They were hallmarks of precise thought and clarity. Only once did he bring a note to class. We were studying the Ising model, and the lecture ended with a very complicated equation. He somehow managed to find a little sliver of paper (he never brought any to class) on which he wrote the equation. He brought the same piece of paper back to class the next time, wrote the equation on the blackboard, and started from there. My daughter got her bachelor's degree in chemistry from Cornell in 2002, and while I was at Cornell for that event, I told Professor Widom this story. He had a better version, which another student had once told him. On the last day of classes he always invites all the students in his class to his house for sherry. In this version of the story, Professor Widom went the entire semester without bringing a note to class, until the last day. On that day he brought a little piece of paper to class with his address on it, so that he could write it on the blackboard and let everyone know where to go.

After leaving Cornell in the fall of 1973, I returned to the Bay Area. Connie had a job offer here, and I love San Francisco. In addition, the prospects for a job for me here were probably as good as or better than anywhere else. Consequently, the decision was a no-brainer. Ultimately, I received a job offer from Sandia in Livermore and started in March of 1974. This was the period of the oil embargo, and Sandia was trying to start a program in combustion. I was to be part of that effort. Combustion was an attractive field for me. One could argue that it is the ultimate interdisciplinary field, requiring knowledge of a variety of topics in chemistry, physics, fluid dynamics, thermodynamics, and mathematics. Moreover, like many other children of the sixties, my formative years were spent believing that science should not be done in a vacuum, but ultimately it should have as its purpose the improvement of the human condition. Working in combustion offered me the opportunity to attack, at a fundamental level, problems related to combustion-generated air pollution. Almost from the very beginning that was the focus of my career.

Historically, Sandia had been an engineering development and support lab, with very little experience in either fundamental or applied research, particularly in Livermore. That made getting started in research relatively difficult, at least for me. However, the situation changed somewhat in October of 1980 with the opening of the Combustion Research Facility (CRF). The new facility brought a steady stream of distinguished visitors to Sandia. These visitors kept everyone abreast of a wide variety of research in all aspects of combustion. Among those visitors who either came to the CRF on a regular basis or for an extended period of time were Jürgen Warnatz, Jürgen Wolfrum, Bob Bilger, Graham Dixon-Lewis, Jim Keck, Tom Bowman, Wolfgang Kollman, Forman Williams, and Owen Smith, among others. In retrospect, the CRF appeared to be the center of the combustion universe in the 1980s and early 1990s.

Another important event was the beginning of the Department of Energy's fundamental chemical physics/combustion program, funded through the Office of Basic Energy Sciences, Division of Chemical Sciences. It is generally agreed that this program began at a contractors' meeting held at the Howard Johnson's in Dublin, CA (near Livermore), in the fall of 1978. This program has brought together a large number of talented scientists, who meet annually at the contractors' meeting, with a focus on the chemical physics of combustion. So far the program can count two Nobel Prize winners among its participants (Yuan Lee and Bob Curl). This program has been an invaluable source of inspiration (not to mention financial support) for me over the years.

The 1970s and 1980s were difficult times for getting jobs in the sciences and engineering. As a consequence, the Sandia combustion program attracted a large number of young scientists and engineers that it otherwise might not have been able to hire. These people are primarily responsible for the quality of the research at the CRF during the 1980s and early 1990s; a large fraction of them went on to tenured faculty positions at major research universities. Included in this group are Bob Kee (the George R. Brown Distinguished Professor at the Colorado School of Mines), Reggie Mitchell (Stanford), Bob Dibble (Berkeley), J. Y. Chen (Berkeley), Mitch Smooke (Yale), Bob Cattolica (U. C. San Diego), Bob Hurt (Brown), and Chris Edwards (Stanford). These people have generally continued their success at these other institutions.

Whatever success my own research has enjoyed is due to a number of fruitful collaborations. I do not want to name everybody I have ever worked with (there is a list of collaborators elsewhere in this volume), but I do want to single out four people: Bob Kee, Carl Melius, Peter Glarborg, and Stephen Klippenstein.

Bob Kee and I developed a collaborative relationship that began almost the first day I arrived at Sandia and lasted for about twenty years. Bob and I shared the opinion that combustion, and chemically reacting flow in general, could and should be done with real chemical kinetics models. Bob felt this so strongly that he thought that others should have the opportunity to do such modeling as well. Thus he became the driving force behind CHEMKIN. Due to Bob's efforts CHEMKIN has become the defacto standard software for modeling chemical kinetics in combustion, as well as some other fields. Its impact on the combustion field is hard to measure.

Carl Melius and I shared the vision that theoretical chemistry could have an enormous impact on combustion. Carl's development of the semi-empirical, BAC-MP4 electronic-structure method was an important milestone in making this shared vision a reality. I believe our vision has been borne out. Theoretical analyses of elementary reactions in combustion are now commonplace, even if they are frequently strong on the electronic structure and weak on the dynamics (a pet peeve of mine). Even many experimental papers interpret their results in terms of a potential energy surface obtained from high-level electronic-structure calculations. This is certainly an encouraging trend.

Peter Glarborg arrived at Sandia as a visitor in the autumn of 1984, while he was still a graduate student at the Technical

University of Denmark. He was interested in modeling some well-stirred reactor experiments concerned with prompt NO and hydrocarbon/nitric-oxide interactions. His enthusiasm was contagious, although he was a terrible pest. I remember repeatedly going over with him the results of his calculations and suggesting other things he might try to shed light on the problem, expecting that my suggestions would occupy him for at least two or three days. Invariably he came back to me with the new results in two or three *hours*, a testimony to both his intellect and persistence. Luckily for me, Peter and I have had a number of other, equally stimulating collaborations over the years.

Perhaps the most productive period of my career was the five-year period, 2000-2005, when Stephen Klippenstein worked at the CRF. Stephen is a brilliant and hard-working theoretical chemist. According to ISI Web of Science, we have co-authored thirty papers together, virtually all of which were either written or published during that five-year period. My collaboration with Stephen has given me the opportunity to attack and solve problems that ten years ago I did not believe would be solved properly during my career. This has been an exciting and fruitful time for me; I hope it has been for Stephen as well.

Connie and I have two grown children: Abigail and Nathan. Both are budding scientists. Abigail got an AB degree in chemistry from Cornell and is almost finished with her Ph.D. at Berkeley. Unlike her father, she has an experimental bent. Nathan got his AB degree in mathematics from Princeton, where he also played baseball (he shares his father's enthusiasm for sports). He is currently a graduate student in physics at U. C. San Diego, doing research in cosmology. I hope they enjoy their research as much as I have so far. I still enjoy it and hope to make some more contributions in the near future.

James A. Miller