Text of the invited talk given at the CFX conference on CFD
29 November 2005

Dear friends of CFD,

I am pleased to have received this invitation of Haridoss to speak to you on my experiences and make some relevant observations in the area of CFD.

In the mid-sixties when I worked for my Ph. D on ignition-extinction problems in laminar unmixed flames, solving problems in combustion meant for us in India solving ODE's with single step reaction kinetics. An era when understanding combustion process was in infant stages with high activation energy asymptotics considered highly respectable, pursuing analytical solutions was not out of vogue. Checking calculations meant use of merchant calculating machines. Use of similarity principles, treating stagnation point configuration that allowed such simplification, making predictions that would be more qualitative because kinetics is not founded in realism was the order of the day. Even such research was applauded!

It was clear to me that if predictions on ignition-extinction problems had to derive respectability so as others like flame speed or the burning velocity, a fundamental combustion parameter, there was no escape from full chemistry calculations. Full chemistry description was getting refined through the seventies and therefore it would be ideal to work on full chemistry problems. Premixed flames appeared more appropriate since diffusion flames are less dependent on chemistry for the rate of combustion. From this, started the code development for premixed flames that adopted a more straight forward unsteady approach than the more cumbersome steady state approach used in the USA. Several Ph. D theses were done using this code meant for full chemistry and one outstanding contribution was a **definitive conclusion that adiabatic flames do not have a flammability limit** (Dr. Lakshmisha's thesis). Flammability limits required invoking an irreducible minimum radiative heat loss. Dealing with spherical flames that was a subject of study for a few years could still be ODE based (as you can appreciate). Much was learnt about how heat release occurs in a premixed flame, how stretch effects have complex relation with chemistry, etc.

Time came to move on to 2D. My colleague, Prof Paul wrote a 2 D reactive fluid dynamic code and the first case that was tested was stretch effects on a Bunsen flame. Since there was competition for work in this area, application for this code was found in the area of Ammonium Perchlorate (AP) – Polymer sandwich propellant combustion that required tracking a burning surface and observing the variation in combustion process due to the distortion in the surface. This research forming Dr. Ramakrishna's thesis had a test of confidence in CFD. Solving two momentum equations with energy and species conservation equations using 3-step chemistry with along with a pyrolysis law for AP surface decomposition and unsteady condensed phase were the substance of the problem. Computer solutions with the known chemistry parameters from the literature always went chaotic. Code was suspected. This suspicion proved incorrect and the non-converging nature of the solution persisted. After much soul searching, the simplified problem of AP combustion was run in 2 D mode. Non-convergence of solution persisted. It was clear that the non-convergence of the full problem must have been related to some instability. Linear instability solutions from literature were then examined; these clearly showed that for the chosen parameters that were standard in the literature for over thirty years and used by all stalwarts, the solution of the full unsteady problem was unstable and this feature had bypassed all the stalwarts because they never treated the problem fully and when a few treated the problem fully, did not analyze what they found clearly, and bent other features to somehow show a steady result – great science by stalwarts!. Then onwards, the pathway for Ramakrishna was clear but not necessarily bright. The physically observed steady combustion process implied that the chosen parametric values for a crucial parameter, namely, the activation energy for pyrolysis was incorrect. Efforts were put in to determine this parameter consistent with other experiments and the observations of AP and AP-sandwich combustion. A paper was written and sent of to a journal. One reviewer, from what we deduced, as a stalwart was highly caustic arguing how a new study that departed in its choice of parameter from those of the stalwarts could be correct at all!. It then took two years, spirited defense at an international conference by Ramakrishna, showing up the presence of this instability in others' calculations not adequately recognized, and arguments with several scientists to remove the blocks in the minds of a few scientists and the editor of a journal for the important finding to see the light of the day. The central message from this struggle is that it is important to have faith in CFD for oneself, that too of a substantive nature for ensuring that others respect your findings.

On the subject of faith in CFD, I must relate my recent experience. I attended an important review meeting of a major project as a member. This meeting was chaired by a very distinguished accomplished head of a major national project with CFD-India's who-is-who all being there as members. Many external flow simulations were presented with some good comparisons and some not-too-good comparisons. Some noises ware made, but results were accepted broadly. There was then a presentation on **experiments on air-intakes** by a distinguished scientist. Till that point, the presentations showed results of calculations and experiments, but the air-intake results had no comparisons with calculations. I asked how come, there are no calculations. There were responses of a bewildering kind. One distinguished person stated that no internal flow calculations of air intakes had been made and it is difficult! Other defenses from stalwarts were that experiments showed the truth and should be trusted and the lack of calculations for air intakes was an acceptable state. I must tell you, that I was completely non-plussed, for, I had not bargained for a sudden nose-dive in the quality of appreciation among distinguished people. The central message that I got was that CFD people doing external flow had no feel for internal flow problems – why I do not understand. The equations are the same, the governing phenomena will have one key feature that is different. Viscous dominated features like separation, shock-boundary layer interaction issues, mixing layer-boundary layer interaction can be far more severe in internal flows and it is perhaps true to say that all the modeling aspects have not been understood. Even so, some broad features can usually be predicted well or the differences tracked down to specific features of the model. For instance, it is generally known that k-ε turbulence model does poorly in recirculating flows and flows with separation. But this does not mean all aspects of predictions will always be poor. In any case, of the several classes of experiments done, some that would be straight forward could be simulated well and reasons for poorer comparisons, if any can be tracked down. Nothing of this class could even be discussed in the meeting.

This brings me to the next question: Should comparisons of predictions with experiments mean that experiments are always to be treated as reference for comparison. Rather are experimental data holier than computational results. Most often the undercurrent of thinking in the mind of an average computational man is to somehow show that comparisons are good, for otherwise people may suspect the quality of computational results. I think, if the person who has computed has taken adequate grid resolution, used the appropriate boundary conditions, the person must have confidence in the results and there should be no hesitation to begin to doubt the experimental results. One should then go ahead and examine the experimental technique, the accuracy of the measurements, back ground of the earlier work of the investigators, etc to ensure the integrity of the experimental data. This might reveal aspects to support the suspicion of the quality of experimental data. One could then bring these out into open for clear discussion. I had two experiences in this direction.

I was studying two decades ago a problem known as erosive burning of solid propellants. I had constructed a theory and this was published. Some years ago, I revisited the problem. Lot more data was now available on many propellants and some reviews too. The reviews seemed shallow and the data presentation technique was designed to avoid controversies even if one existed. I used some data on the same propellant by two different investigators and cast them on a single plot using non-dimensional coordinates. These showed clear differences. Then I put together lot of other data on the same plot. It looked as though the differences that were seen between vastly different propellants were no more than for the same propellant by different investigators. The conclusion was that this would be the irreducible minimum difference that one could not avoid even with best of intent. And, if so, no more experimental work need be done and all the data fitted into a single universal curve (the work published with my colleague, Prof. Paul). Perhaps one should be brave to suggest this. And many superficially minded people might even debunk my conclusion. It is only the carefully minded person that can see the gravity of the conclusion – no more experiments are needed!

More recently I had another strange experience of people wanting to avoid controversies even when they are very visible and are pointed out. One of our students Sudarshan Kumar Vatsayan (currently Dr. Sudarshan Kumar, V) while was working on flameless combustion was examining lifted gaseous flame data. Lifted flames have occupied the interest of combustion scientists perhaps, to an obsessively large degree. There were experimental data on the same fuel-oxidizer combination by two different authors. The experiments were extremely simple – determine the lift height under different flow rates of fuel and oxidizer. Here again, the results of two different authors for the same fuel-oxidizer combination showed significant differences. Communication with the authors themselves and a few others showed an unacceptable scientific attitude – “I swear by my results. I will not comment on others’ results” – truly strange. There was no other way than to publish the results as they were. They even have got published with no comment from any reviewer or other authors. We perhaps must allow time before somebody adequately brave takes up the issue.

The summary of all these experiences is that we should work hard to build our own confidence in what we do – through careful checks, responding to criticisms through additional work, if necessary, or whatever it takes to be sure of oneself. By building confidence in CFD (not over-confidence), we will help the designers and some times the experimenters too – for, they do not usually have the privilege of seeing all the details of the flow field that CFD will provide. Experimental combusting flow mapping is far more difficult.

I think I have said all that I needed to say. I hope I have said things of which some might be a part of your experience. Thank you for your patient listening.