GUEST EDITORIAL

Simulation Apps Bring Us Closer to Mars

by **JIM KNOX, MARSHALL SPACE FLIGHT CENTER, NASA**

My work with mathematical modeling and computer simulations began in earnest in 1987 when I signed on with the National Aeronautics and Space Administration, better known as NASA. At the time I was developing computer simulations to support the design of carbon dioxide (CO_2) removal systems for the International Space Station (ISS) life support system. CO_2 is a human metabolic waste, produced at a rate of a kilogram per day per crewmember. CO_2 must be removed from the crew cabin, as it will quickly become detrimental to crew health. The systems used to remove CO_2 are typically based on sorption processes, which include complex interactions of heat transfer, mass transfer, and gas flow through porous media. At this time, there were no commercial options for solving a set of coupled mathematical models such as partial differential equations (PDEs); you either force-fit the physics into a thermal analysis package or wrote your own code, complete with discretization, meshing, and solution algorithms. Unfortunately, coding CO_2 removal processes from scratch did not allow an appropriate focus on the challenging yet crucial task of understanding and capturing the underlying physics via appropriate mathematical models. Configuration control was often simply ignored due to tight schedules, resulting in a code that would be quicker for a second party to rewrite than modify.

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In the early 2000s, I decided to move CO_2 removal simulations to a platform with built-in meshing, solvers, and postprocessing capabilities, and that could solve user-defined multiphysics PDEs. The program chosen to meet these needs was COMSOL Multiphysics®. Along with freeing the engineer to focus on the underlying physics, a degree of configuration control was automatically achieved via a consistent user interface, thus allowing COMSOL users to share computer models. My team has developed simulations that are already providing a valuable debugging capability for the ISS CO_2 removal system, and will provide guidance in upgrades to that system.

As NASA looks to the next phase of human space travel, first to the vicinity of Mars, and then eventually to the Mars surface, the need for robust and efficient systems takes a quantum leap. Unlike on ISS, resupply is unavailable, and early return is impossible. Design of CO_2 removal systems thus requires a new degree of optimization, including selection of adsorbents and sorbent processes.

One facet of my current position, guiding the maturation of spacecraft CO_2 removal technologies for NASA's Advanced Exploration Systems program, is keeping abreast of parallel developments in CO_2 capture and storage. While listening to a speaker at a recent conference, I was struck by his conclusion: For this complex technology, standard figures of merit cannot be used to optimize the processes involved. Rather, computer simulations that capture the key physics of the process, including coupled heat and mass transfer in porous media, must be applied. A large number of parametric simulations are required to converge on the optimal solution. Parametric testing could also be employed, of course, but would be prohibitively expensive and time-consuming, severely limiting the number of options that can be explored. Multiphysics applications have made great strides in solver robustness and speed. However, to accelerate 1D system simulations and enable multidimensional modeling of full CO_2 removal systems, further improvements in robustness, execution rate, and memory usage are highly desirable future developments.

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One feature that can be applied now to increase the execution rate of parametric studies is the Application Builder in COMSOL Multiphysics®. After verification of a CO_2 removal simulation against test results, the configuration can be locked down and a simulation app distributed to multiple users for parallel parametric studies. Examples of parametric variables include sorbent selections, fixed bed size, cycle times, and flow rates. The recent development of the Application Builder is very timely, as it will seamlessly facilitate this process.

In summary, early investigation of COMSOL as a platform for parametric studies towards maturation of spacecraft CO_2 removal systems appears very promising. The Application Builder will provide the means to distribute the workload to many individuals. With this approach, informed selections from a wide range of possible options can be made towards finding the best solution of a CO_2 removal system for the crew traveling to, and landing on, the Red Planet. ❖