Efficient Hydrogen Saturation and Transfer Rate Simulation in Metallic Rods

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Abstract: Lanthanum Nickel ($LaNi_5$) has been shown to be an excellent candidate for efficient hydrogen storage and transportation. Experiments with these metallic rods have shown steady and contaminant-resistant absorption and desorption rates at relatively low temperatures (300-325K) [1]. Modeling of these and other rod's behavior in hydrogen rich environments over any significant time period or accuracy range have taken enormous computing power and wall-time, limiting the number of simulations for possible modifications to the $LaNi_5$ composition and other alloy testing. A parallel programming approach was used to drastically reduce the time necessary to model the hydrogen saturation at different radial distances from the edge of a $LaNi_5$ rod, as well as the absorption rates at the same points. Fortran 90 programming is being used in conjunction with MPI conventions on the LONI computer cluster to reduce the computing time from 32 hours to ~2 hours.

Keywords: Desorption, Lanthanum Nickel, Hydrogen Saturation, MPI, LONI

1. Introduction:

Hydrogen power was once heralded as the next generation in power production and liberator of nations from foreign fuel sources, but the fruition of such promises has been slow-coming in the past decade. Thus far, net energy production from hydrogen sources do not account for the amount of energy necessary to produce and transport the hydrogen itself, and therefore such generators are currently used only in large industrial and corporate situations, namely as reliable backup generators [2]. Cost-efficiency is also another necessary consideration that still has not met target ranges, both in storage options and within generators themselves. Four options present themselves for transportation of raw hydrogen, namely its gaseous and non-compressed form, liquid phase, compressed gas, and metallic hydride storage. Taking hydrogen in its gaseous form at atmospheric pressure presents multiple problems, from unreasonably large and costly tanks to high Hindenberg-type safety issues. Pressurizing the gas means very costly thick tanks and still presents safety issues. Liquefying hydrogen

and keeping it in this state during transport is extremely costly and reduces energy efficiency of production, as well as limiting the temperature range of generators. Metallic hydrides present a feasibly viable option for transport if low-cost metal alloys can be found and release rates can be effectively predicted. It is the purpose of this study to effectively map the density of hydrogen in these metallic rods and used such information to predict desorption rates at given initial temperatures. Our current serial code takes approximately 32 hours to run through its 10,800,000 time-steps to model three hours' worth of hydrogen absorption from a metallic rod. Distributing this process with MPI parallel programming would allow for tests of multiple hydrides and longer periods with less computational cost. Complexity arises in this approach through managing communication between processors and ensuring that the correct information is supplied to all processors in order to run calculations and then collected in meaningful configurations, which further must be optimized to ensure that this communication time does not negate the efficiency gained from distributing the calculations.

2. Procedure:

Extensive knowledge of Fortran 90, especially of the array features, was first necessary in order to begin writing basic functions to be integrated into the programming scheme. Basic Laplacian matrix programs using 60 by 60 meshes utilizing Jacobian iteration techniques were first formulated. Such a method's main computations took place in utilizing two DO-loops going from the 1^{st} to 59^{th} grid point (ie. the interior points of the matrix) and forming an two-dimensional array derived from ¼ of the summation of its surrounding points. The serial program consisted of 62 lines of code and was easily modified for larger meshes. Termination of this program relied on the difference between subsequent values at a specified grid point; if the difference between a value of the matrix between timestep *n* and *n+1* fell underneath a specified tolerance, the program was terminated. Parallelizing this program utilized the MPI_REDUCE and MPI_BCAST functions in order to consolidate this difference information and ensure that the maximum difference in subsequent time-step values was measured against the set tolerance. Results of said programs (see section 3) suggest that similar techniques when applied to larger and more computationally varied situations could greatly reduce walltime needed for calculation of a hydrogen storage scheme. Such a program was developed that took the initial specific heat of both hydrogen and the metallic rod, their thermal conductivities, epsilon porosity, heat of formation for the reaction, permeability of the porous rod, dynamic viscosity of the hydrogen, and respective initial densities and temperatures and used said information and Jacobian iteration techniques it model the saturation of hydrogen at different column mesh points corresponding to radial distances from the edge of the rod. To split array computations between processors, two separate numerical schemes were developed to account for computations including and excluding the boundary points, respectively. For calculations involving boundary points, the columns were broken up in the following manner: *DO j = myid*(Nz/nprocs)+1 , (myid+1)(Nz/nprocs)*

Where *nprocs* is equivalent to the number of processors being utilized and *myid* gives each processor a rank from zero to *nprocs*-1. Inspection confirms that this scheme successfully iterates all points between j=1 and *Nz*. In such a scheme each processor was responsible for calculating all of the rows for the columns it was assigned. For interior point calculations, such a basic scheme was not possible to include all mesh points between j=2 and Nz-1, so an IF-THEN-ELSE structure was used:

if (myid .eq. 0) then j=2,Nz/nprocs
else if (myid .eq. nprocs-1) then do j=(Nz/nprocs)(nprocs-1)+1,Nz-1*
else do j=myid(Nz/nprocs)+1,(myid+1)*(Nz/nprocs)*

By isolating both the first and last processors, which each are assigned one less computation than the other processors, the other processors could use the same scheme as before. The final mesh was 40 by 40, yet was programmed in such a way as to allow for differing lengths and widths of the rod.Our tested model had a rod length of .05 meters and a diameter of .03 meters. After such modifications and MPI communication devices were added to the program, the programmed totaled 2419 lines.

3. Results and Discussion

For our original test Laplacian 60 by 60 matrix the tolerance was set to 1E-5, which ran through 9042 iterations before terminating after .4 seconds. The parallel version of this test program, again set to a tolerance of 1E-5, completed in .0735 seconds, yielding a 544% speed increase. Buoyed by such results, comparable time increases were sought in measuring the effectiveness of Lanthanum Nickel as a viable hydrogen storage option. The serial version the developed code ran for upwards of 32 hours and stored data on the density of hydrogen in the rod, desorption rates, hydrogen pressure, velocity of the hydrogen, and temperature of the solid at ten minute intervals.

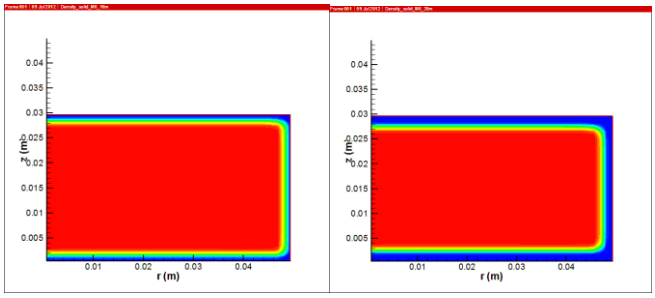


Fig.1

Density of Hydrogen (kg/m^3) at 10 and 20 minutes, respectively. Red corresponds to high concentrations of hydrogen, blue to low. Ranged between zero and 360 kg/m^3. X and Y axes map the z and r components, respectively.

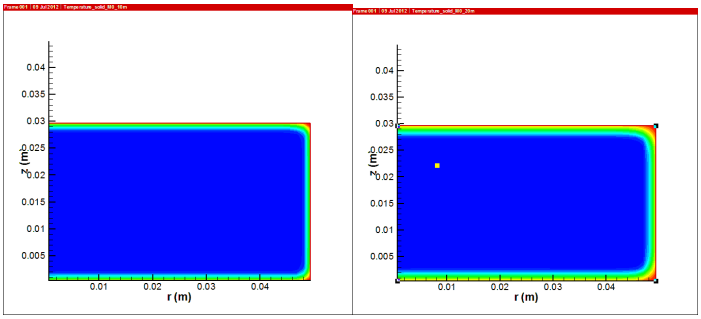
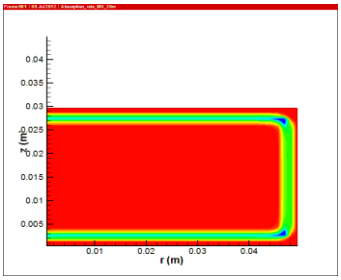


Fig. 2

Temperature (K) of Rod at 10 and 20 minutes, respectively. Red corresponds to high temperature, blue to low. Ranged between 297 and 317 K. X and Y axes map the z and r coordinates, respectively.

Fig. 3 

Desorption of hydrogen (kg/sec). Maximum desorption at .206 kg/s. X and Y axes mark height and radius components, respectively.

Because of the consistently low temperatures within the rod at high hydrogen concentrations, Lanthanum Nickel is modeled to be much safer than other means of hydrogen transport. At a maximum concentration of 360 kg/m^3, hydrogen packed within $LaNi_5$ is at the upper range of hydrogen saturation among other meta l hydrides [3]. Low surface desorption results in highly controllable reactions, though tests are still being done at higher initial temperatures to ensure this phenomenon is consistent. Though data has not yet been produced from a parallelized version of this code, this week will mark first tests of MPI implementations.

4. Conclusion

Lanthanum Nickel appears to be in the top range of candidates for hydrogen storage in metal hydrides. If MPI implementations can be successfully run on the LONI supercomputer cluster, this program could be used to model both different initial conditions and longer time periods for $LaNi_5$ but also can be used to get precise measurements for other metal hydrides without high computational costs. This technology will be beneficial in predicting which metals can reach standards of concentration of hydrogen per weight of rod to allow for cost-effective storage and transport of hydrogen.

5. Acknowledgements

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6. References

[1] Flanagan, T.B. and S. Tanaka. “Hydrogen storage by LaNi5 - Fundamentals and applications” http://adsabs.harvard.edu/abs/1977empe.symp..470F. Accessed July 8, 2012.

[2] http://batteryuniversity.com/learn/article/fuel_cell_technology. Accessed July 9, 2012.

[3] Ragheb, M. “Hydrides Alloys for Hydrogen Storage”. https://netfiles.uiuc.edu/mragheb/www/NPRE%20498ES%20Energy%20Storage%20Systems/Metal%20Hydrides%20Alloys%20for%20Hydrogen%20Storage.pdf. Accessed July 9, 2012.