Metal-Water Reaction Model Improvements

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Outline

- Background
- Discussion of Work Performed
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- Summary

Background

- This work is based on User Problem #10060. This user problem requested additional modeling capabilities for the metal-water reaction model.
- INL expanded applicability of the metal-water reaction model for all geometry types for the metal-water reaction model. Previously only cylindrical heat structures could be used.
- It was also required that parameters used by the metal-water reaction model be allowed as user-input for model flexibility (i.e. allow other materials to be modeled in addition to zirconium).

Discussion of Work Performed

1. Fixed the metal-water reaction failure in the F90 code.
2. Modified the 1CCCG003 card to allow various user-input parameters for the metal-water reaction model.
3. Modified the reaction depth and heat generation equations to include rectangular and spherical heat structures.
4. Modified the output file to include the heat generation due to the metal-water reaction, and add a minor edit variable that allows the heat generation to be plotted for each heat structure.
5. Verification testing was performed using the installation, developmental assessment, and model specific problems. This testing was performed for both Linux and PC platforms.
6. Institutionalized (modified the manual, submitted, implemented and tested updates in the mainline code).

Task 1

- The first task required that the error in the metal-water reaction be corrected. This error was reported as user problem #10068, in which a problem failed when the metal-water reaction model was used.
- There were two conversion errors in the metal-water reaction model.
  - Variable ‘gprinc’ was incorrectly set in subroutine HT1INP.
  - Variable ‘qdo’ was incorrectly set in subroutine HT1TDP.
- These two errors were corrected, and the metal-water reaction model now obtains results similar to previous versions.

Task 2

- Task 2 required the modification of the 1CCCG003 card to allow various parameters to be read. The new parameters are:
  - Material density (W2)
  - Activation energy (W3)
  - Reaction rate constant (W4)
  - Reaction heat release constant (W5)
  - Molecular weight of cladding (W6)
  - Molecular weight of reaction product divided by Word 6 (W7)
  - Initial oxide thickness on the “inside/left” surface (W8)
- If the words are input as 0.0, or omitted the default zirconium-steam values are used.

Task 2

- Allowing the user to input the activation energy, molecular weight, and the molecular weight of the reaction product divided by the molecular weight of the cladding were not part of task 2, but were added because these quantities are necessary for calculating the amount of heat released by the metal-water reaction and the amount of gas produced by the reaction for materials beside zirconium.

Task 3

- Task 3 required the modification of the reaction depth and heat generation equations for all types of heat structures.
  - The Cathcart model currently used to calculate the reaction depth equation was developed using cylindrical test specimens, and an equation was not developed for rectangular or spherical heat structures. A generalized equation was not developed.
  - The heat generation equation was developed for all types of heat structure geometries, and logic was added so the correct equation is used in the calculation.

Task 4

- Task 4 required the modification of the output file to print the amount of heat generated by the metal-water reaction. The amount of heat generated was also required to be a new minor edit variable.
  - The heat generated due to the metal-water reaction was calculated for each heat structure geometry type, and was added to the major edit section of the output file.
  - The heat generation due to the metal-water reaction model was added as a minor edit variable ‘htmwrq’.
  - The rate of heat generated was also calculated by dividing the heat generated each time-step by the time-step size. This quantity was also added as a minor edit variable ‘htmwpow’.

Task 5

- Task 5 required verification testing with both the installation test set and the developmental assessment test set.
- Each problem was run in four different configurations – semi-implicit and nearly-implicit time-step advancement and explicit and implicit hydrodynamic/heat structure coupling.

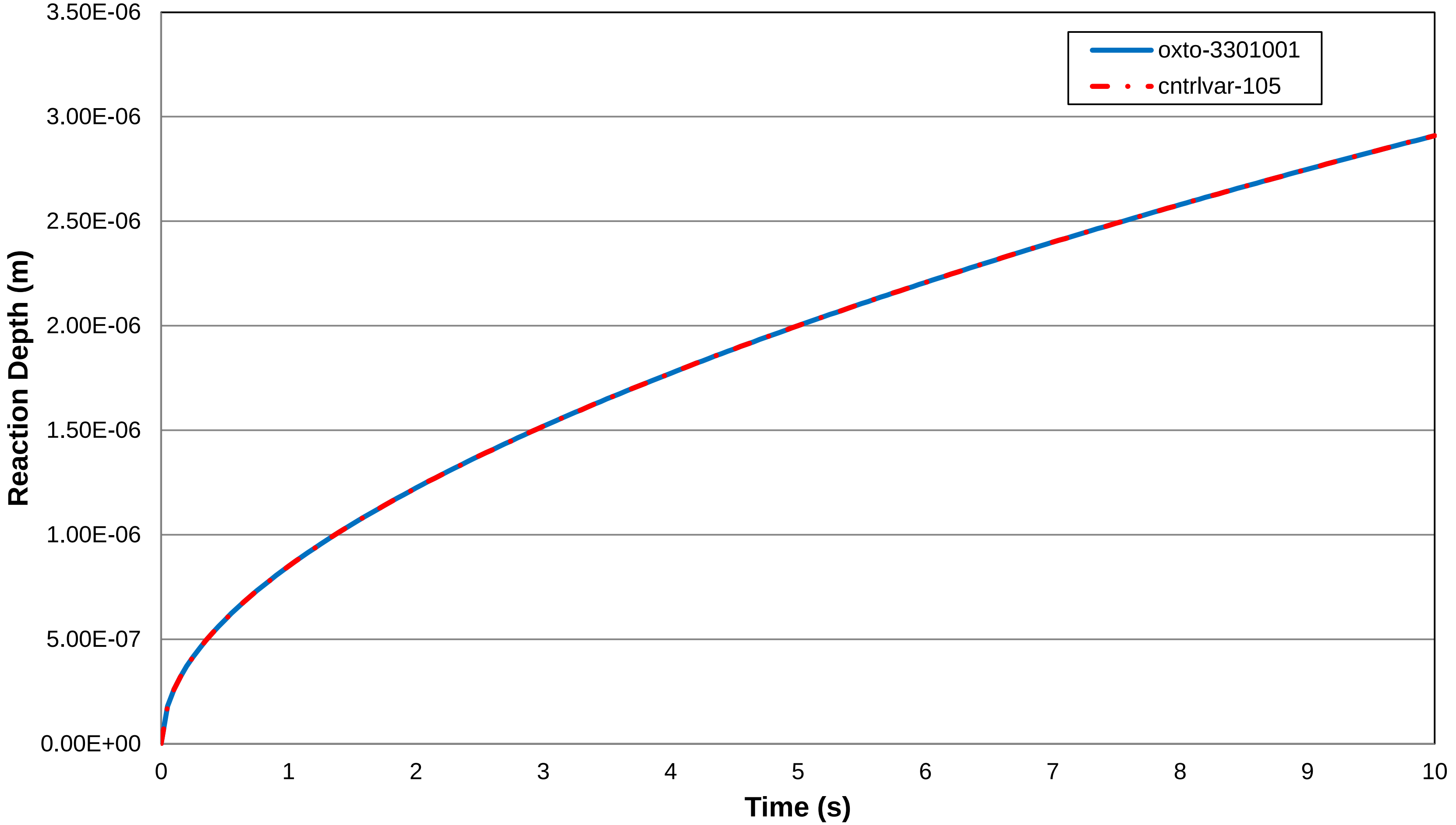
Semi-implicit advancement and explicit coupling	Nearly-implicit advancement and explicit coupling
Semi-implicit advancement and implicit coupling	Nearly-implicit advancement and implicit coupling

- The verification test set was run with and without the metal-water reaction updates. A ‘diff’ was then performed between the two versions revealing no differences. This was as expected, because the metal-water reaction model is not exercised by any of the test problems.

Task 5

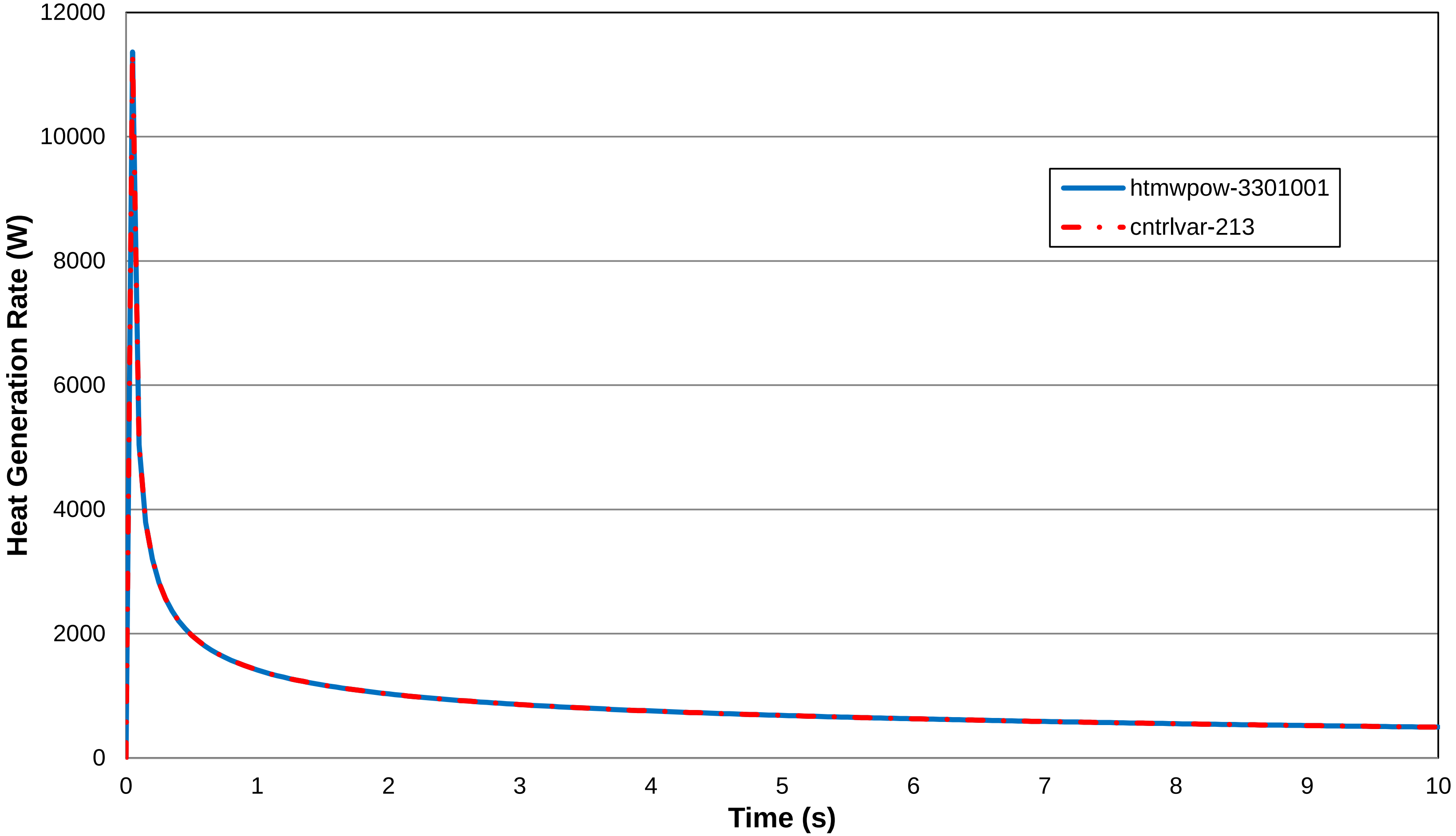
- Test problems were developed for each of the three heat structure geometries.
- The steam and the heat structures were initialized to 1200 K, and there were no heat sources.
- Three heat structures were created to test that the model worked as coded. Using card 1CCCG003,
  - The first heat structure only entered W1
  - The second structure entered W2-W7 as 0.0
  - The third structure entered W2-W7 as values slightly different than the default.
- Control variables are used to calculate the reaction depth and the heat generation rate equations for the three structures. The comparison between the RELAP5 variables and the control variable calculations showed very small differences (largest differences ~1e-9).

Task 5



3.50E-06
3.00E-06
2.50E-06
2.00E-06
1.50E-06
1.00E-06
5.00E-07
0.00E+00
Reaction Depth (m)
0
1
2
3
4
5
6
7
8
9
10
Time (s)
oxto-3301001
cntrlvar-105

Task 5



12000
10000
8000
6000
4000
2000
0
0
1
2
3
4
5
6
7
8
9
10
Time (s)
Heat Generation Rate (W)
htmwpow-3301001
cntrlvar-213

Task 5

- An additional control variable was used to test that the integral of the heat generation rate would equal the RELAP5 variable for the heat generated. This comparison showed a difference of ~13 J for a 10 second transient. When the test problem was run for a longer period of time, the difference was eliminated.

Tasks 6

- To fulfill task 6 the manuals were modified and the coding was submitted and implemented into the mainline coding.

Summary

- The metal-water reaction model was modified and can now be used for rectangular and spherical heat structure geometries.
- The model parameters can be user-input to model reactions in addition to zirconium and steam.
- The testing showed no differences occurred in the installation and developmental test sets with the model changes.
- Verification testing showed that the reaction depth and heat generation are calculated appropriately.

Questions?