Abstract #1738

English

Physics Based Modeling of Thermal ISRU Processes

Over the past three years we have been involved in three different experimental research efforts in the area of asteroid In-Situ Resource Utilization (ISRU). Through these efforts we have demonstrated that application of heat in vacuum can liberate volatile material from meteorites, hydrated terrestrial minerals, and carefully formulated asteroid simulant and we have measure the species and evolution rates of the released gases. In addition we have demonstrated the key elements of Optical Mining™ technology in which intense, focussed light can be used to excavate surfaces will liberating molecularly bound volatiles. In the present work we report on analytical and computational models in which we are able to simulate experimental conditions and validate our understanding of the physical and chemical processes and we use these models to simulate full scale (≈tons per day) asteroid ISRU for the purpose of propellant manufacturing to support a reusable cislunar transportation network.

French

No abstract title in French

No French resume

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Profile of Dr. Joel Sercel

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Biographies

Biography submitted with the abstract

Joel C. Sercel, PhD, is the Founder and Chief Engineer of the Trans Astronautica Corporation (TransAstra), a new kind of aerospace company dedicated to the belief that humanity will thrive as a species once we make the leap and homestead the solar system. With the recent swarm of technological breakthroughs in information systems, manufacturing, sensor systems, and robotics now is the time to move from dreaming about homesteading space, to doing it. TransAstra is building the technology to provide in-space transportation and related services with a fleet of reusable space tugs supplied by propellant derived from asteroid and lunar resources. Our first customer will be NASA, but soon after we will support the new asteroid mining industry for returning valuable resources to the Earth. Space tourism, space solar power, and then space based manufacturing will follow quickly. Dr. Sercel has decades of experience developing advanced technology and innovative products in fields ranging from aerospace and defense to software and robotics. In addition to his private sector work, Joel spent 14 years at JPL and taught systems engineering and space mission and satellite design at the graduate level at Caltech. Dr. Sercel led the conception and definition of the NSTAR ion propulsion system currently in use on the Dawn spacecraft in orbit around the asteroid Ceres. Dr. Sercel received his PhD and master's degrees in Mechanical Engineering from the California Institute of Technology with a doctoral dissertation in plasma physics as applied to space propulsion. His bachelor's degree was in Engineering Physics from the University of Arizona.

Biography in the user profile

Collaborators

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One Dimensional Finite Difference Model of Solar Thermal Asteroid ISRU

- Preliminary Results -

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Coauthors

- Related Experimental Program
  - Leslie Gertsch of MoS&T (PI)
  - Christopher Dreyer of CSM (Experimental Lead)
  - Egboche Unobe of MoS&T (GRA: Experiments and Data Analysis)
  - Angel Abbud-Madrid of CSM (Collaborator)

- Material Properties Analysis
  - Daniel Britt of UCF (Simulant and Asteroid Composition)
  - Leo Pohl of UCF (GRA: TGA and Chemical Reactions)
  - Egboche Unobe of MoS&T (GRA: TGA and Chemical Reactions Literature Analysis)

- General Consultation and Peer Review
  - Diane Linne of NASA Glenn
  - Stanley Love of the Astronaut Office
  - Robert Jedicke of Hawaii IfA

- Phython Code Development
  - Mark Crawford (TransAstra Contract Programmer)

Acknowledgement

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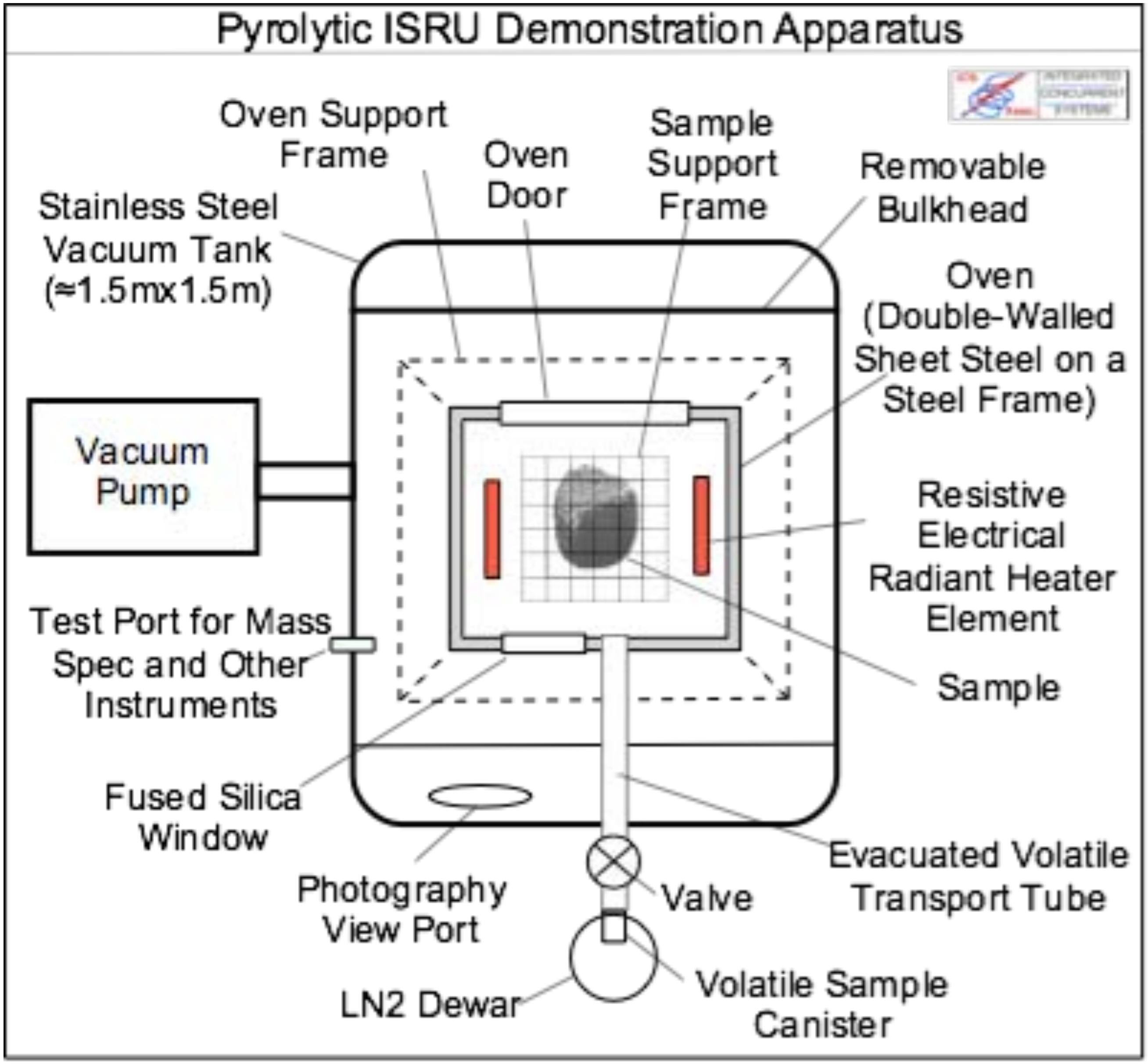
- Additional funding was provided by TransAstra corporation in association with our investors.

Overview

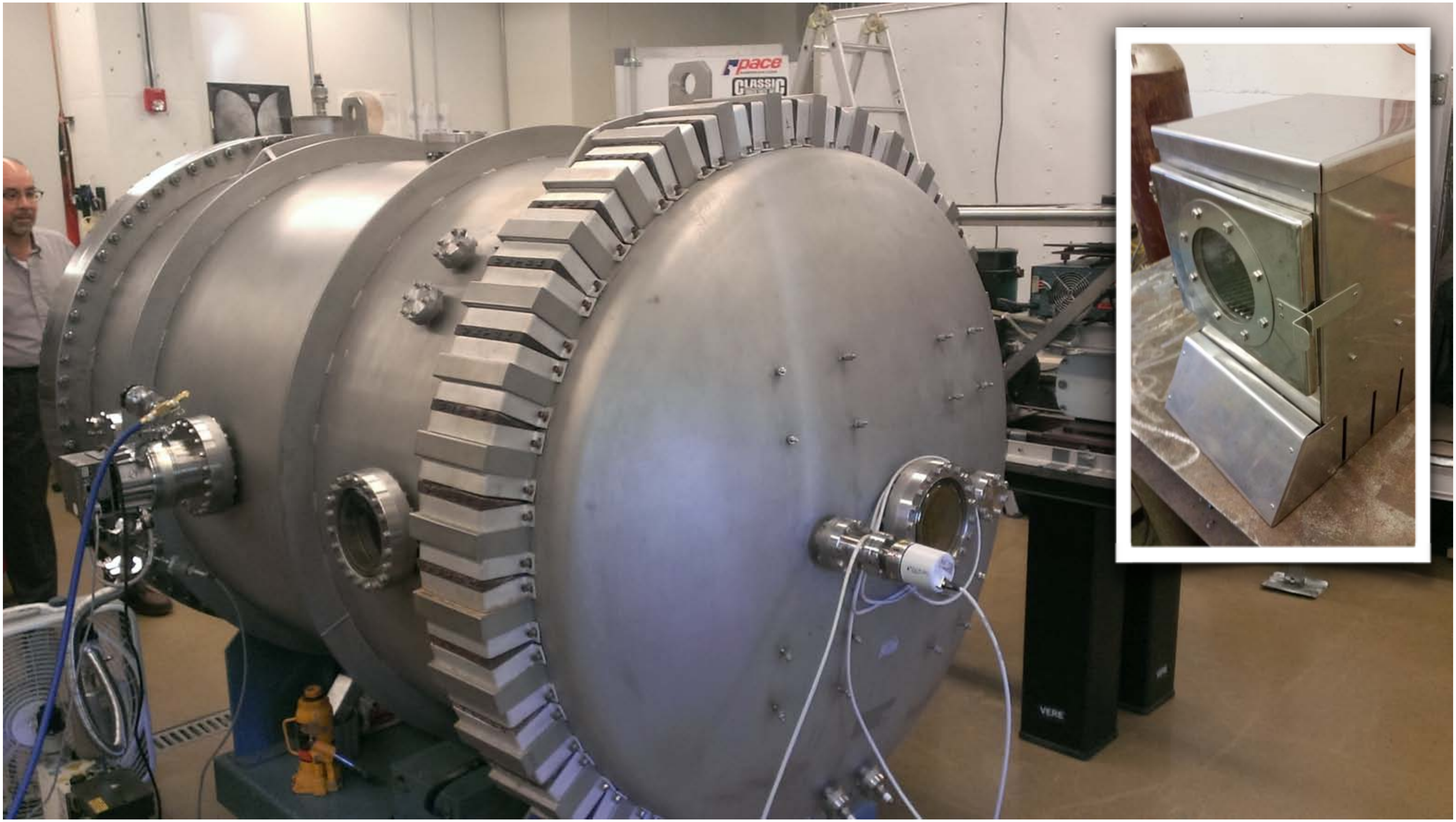
- Motivation
- Physical Model
- Results
- Conclusions
- Way Ahead

Part of a NASA Funded Early Stage Innovation Research Grant



- Year 1 Oven Development and Initial Tests Complete
- Year 2 Experimental Research Program Now Complete
- Data Analysis and Publication Ongoing

Architect: Sercel, PI: Gertsch (MoS&T), Lab: Dreyer (CSM)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CLASSIC
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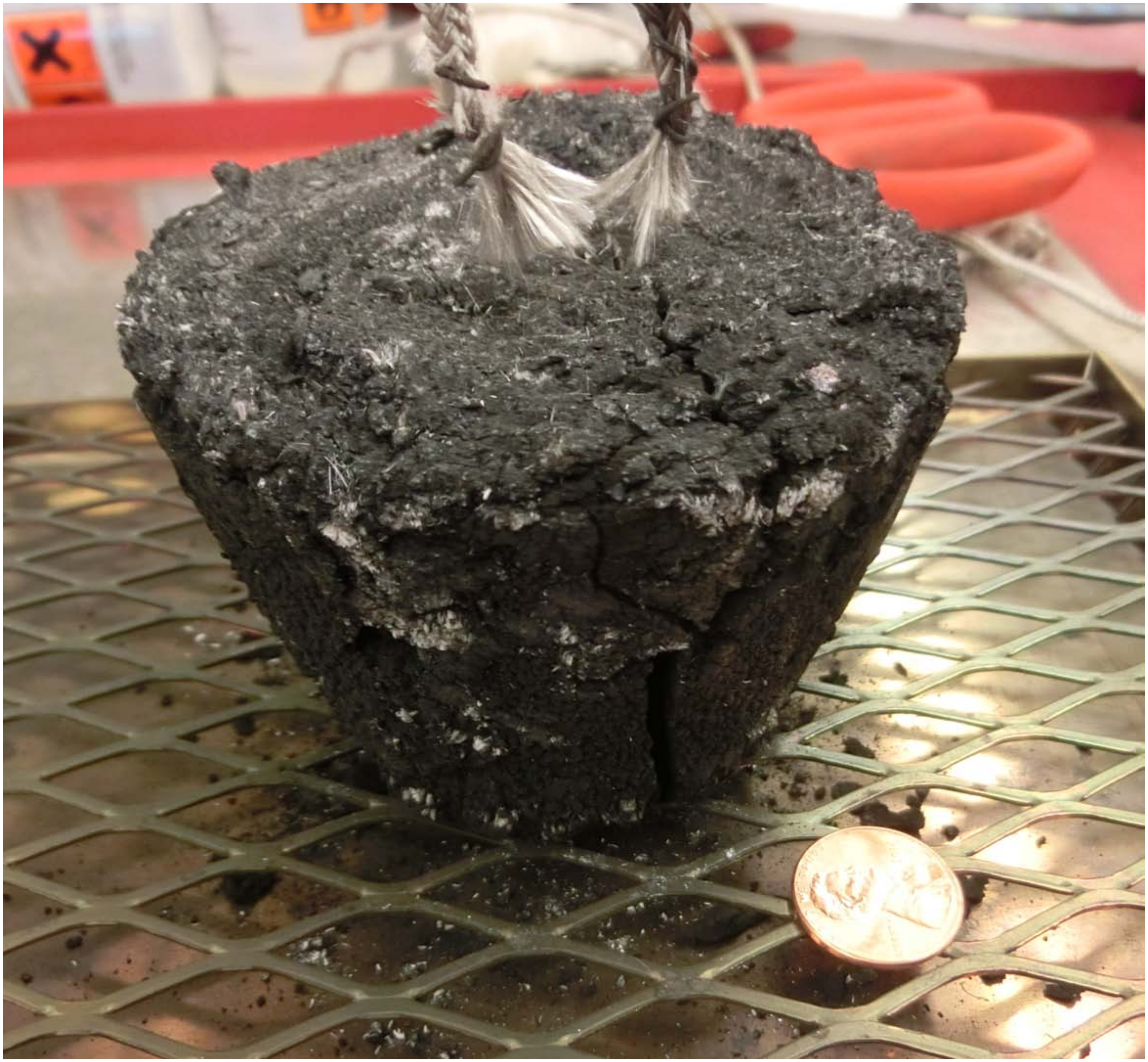
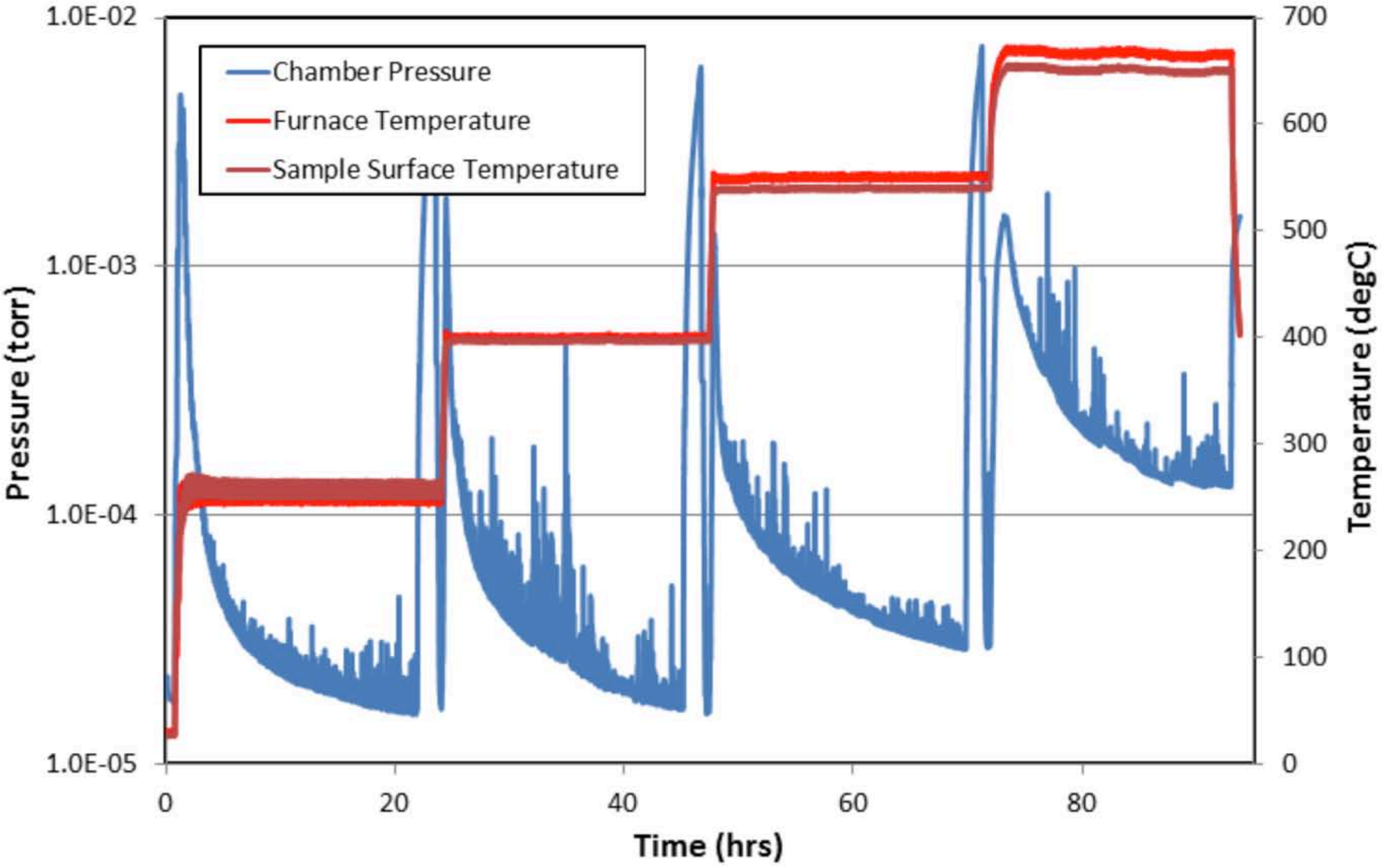


Experimental Data Collected

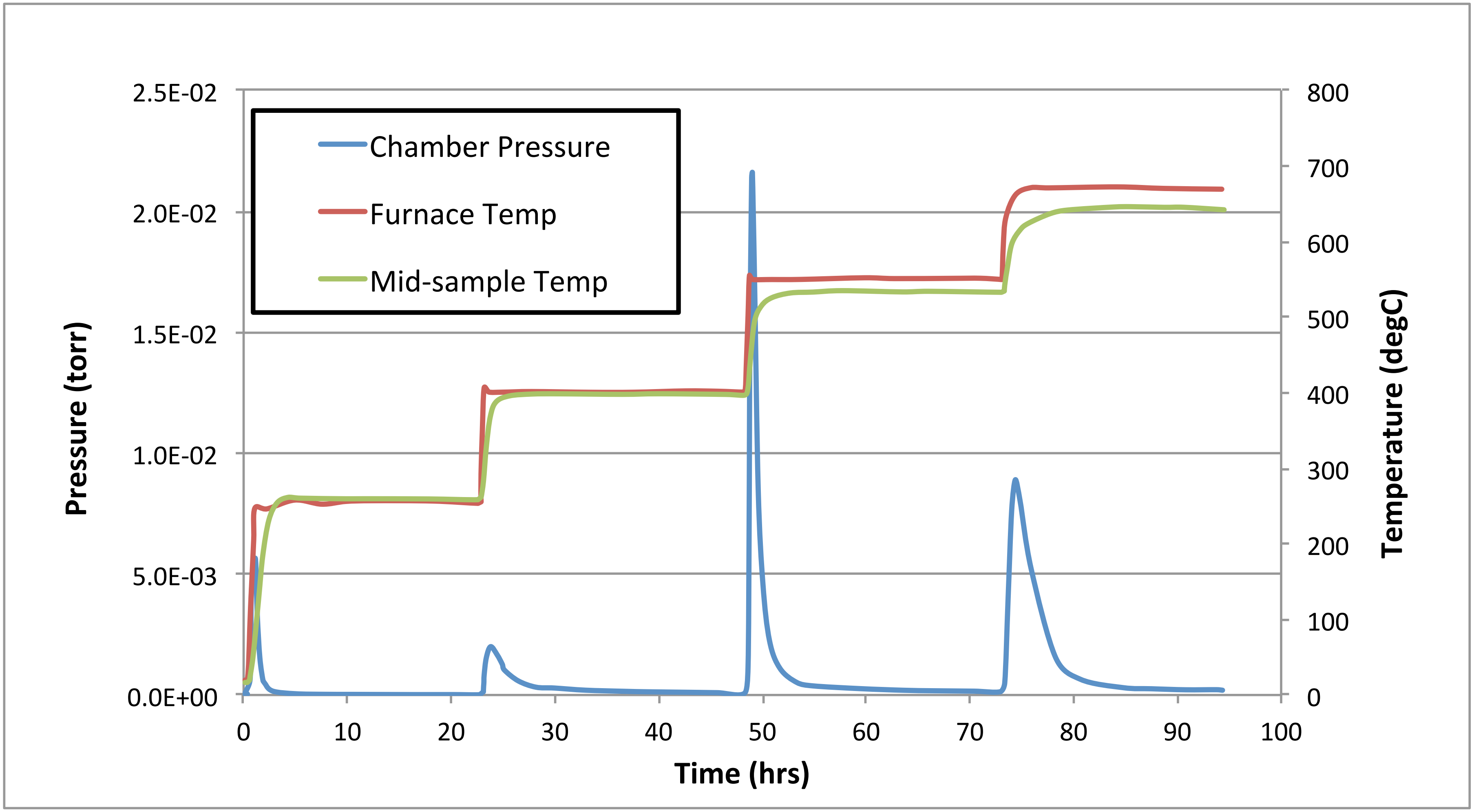
- Before and after physical properties
  - eg., mass lost, color, etc…
- Detailed mass spec of evolved effluents
- Time histories of oven and sample temperature, including centerline temperature in most cases (not for actual meteorite)
- Vacuum tank pressure (which can be used to calculate effluent evolution rate from tank pumping speed)
- Cryotrapped effluent mass for each plateau
  - Chemical analysis pending
- Total ISRU system efficiencies

Multiple Many Day Experiments With Repetition for Simulant Types

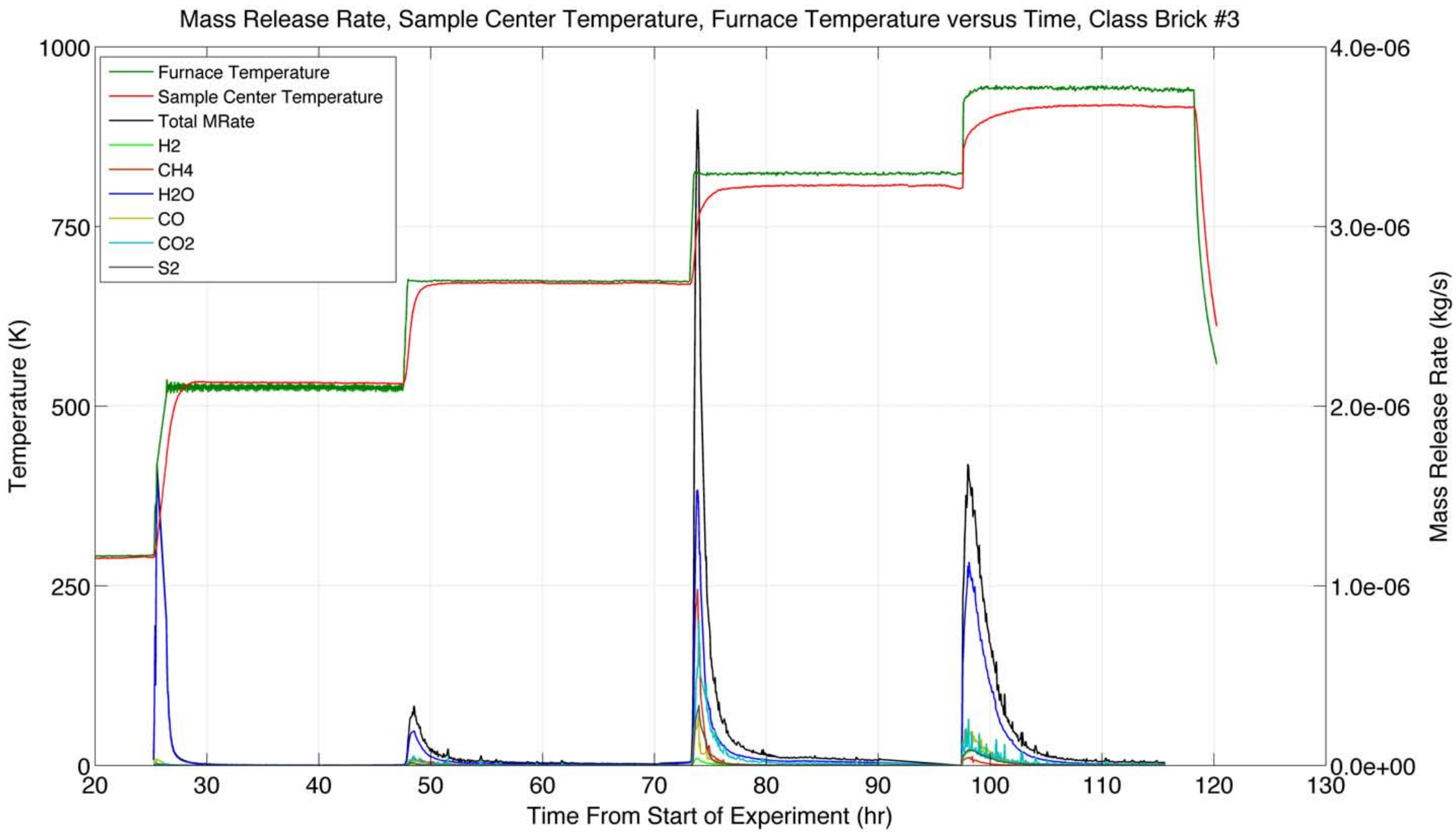
Raw Experimental Results



Cleaned Up But Unprocessed Experimental Results



Example of Processed Experimental Results



Goal of Physics Based Math Model

- Demonstrate understanding of experimental results
  (Have we missed any basic physics?)

- Make practical projections of ISRU performance to evaluate baking as an option

- Develop a code base that can be extended to modeling other resource extraction methods

Content of Model

- Time varying isothermal exterior temperature at T_{hot} simulates oven temperature time history based on measurement

- Initial temperature of all shells T_{cold}

- Heat propagating inward as per heat equation
    - Heat capacities taken from recent D. Britt experimental results
    - Thermal conductivity selected to match observed thermal time constants
      - agree within 20% of published values for meteorites
      - ≈10 less for granular material as expected

- Volatile outgassing modeled as proportional to temperature change within specific chemical reaction temperature ranges (linear gas release response) as documented in the TGA literature for active ingredients/constituents

- Composition of simulants and terrestrial minerals tested modeled based on recipes of experimentalists (all *significant* gas release chemistry included)

- Asteroid ISRU performance and meteorite experiment validation based on known composition of meteorites as representative of asteroid source material mapped to taxonomies

- Interior gas pressure and velocity calculated via Darcy's Law
    - Porosity based on published literature for known meteorites

Typical Physical Parameters

Parameter	Units	Variable Name	Value	Comments
Radius of Target	m	Rt	0.05	Typical of brick tests
Bulk Density	kg/m^3	Ro	2250	Calculated based on size and mass
Void Fraction (Porosity)	fractional	fv	0.2	Typical of brick tests
Specific Heat	J/(kgK)	Ch	800	Typical of brick tests
Thermal Conductivity	W/m-K	k	2	Calculated based on thermal time constant
Thermal Time Constant	s	Tau	2.81E+03	Measured
Initial Temperature	K	Tcold	700	All shells set to this at t=0
Time Steps Per Time Constant	#	Nt	200	Determined with tests to provide numerical stability
Time Step	s	tstep	14.06	Calcuated
Mass of Target	kg	m	1.2	Measured
Number of Shells	#	Ns	50	Assumed
Shell Thickness	m	dR	0.005	Calcuated

Simulant and Meteorite Volatile Sources

Source Mineral	**Mass Fraction of Source Mineral in CI Simulant (brick/granular)**	**Mass Fraction of Source Mineral in CM Simulant (brick/granular)**	**Mass Fraction of Source Mineral in CM Meteorite (Murchison)**	**Mass Fraction of Source Mineral in CI Meteorite (Orguil)**
Atmospherically adsorbed, Preparation process water	0.015 - 0.05	0.015 - 0.05	~ 0.01	~ 0.01
Smectite	0.05	0	0	0
Vermiculite	0.09	0	0	0
Lizardite	0.48	0.22	0.22	0.815
Antigorite	_	_	_	_
Chrysotile	_	_	_	_
Cronstedtite	0	0.57	0.585	0
Vermiculite	0.09	0	0	0
Pyrite	0.065	0.025	0	0
Pyrrhotite (FeSx), assuming x = 1.14, (Harries+, 2013)	0	0	0.029	0.045
Epsomite	0.06	0	0	0
Smectite	0.05	0	0	0
Calcite	0	0.01	0.011	0
Sub-butiminous Coal	0.05	0.035	0	0
Isolated Kerogen	0	0	0.035	0.05

Volatile Mass Fractions In Materials Modeled

Released Gas	**Source Mineral**	**Mass Fraction of Gas Release Per Source Material (kg/kg)**	**Yield from CM**	**Yield from CI**	**Yield from CI Simulant**	**Yield from CM Simulant**
H_2O	Atmospherically adsorbed, Preparation process water	1	0.01	0.01	0.015 - 0.05	0.015 - 0.05
H_2O	Smectite	0.05 - 0.15	0	0	0.0025 - 0.0075	0
H2O	Vermiculite	0.07 - 0.09	0	0	0.0063 - 0.0081	0
H_2O	Lizardite	0.12 - 0.13	0.0264 - 0.0286	0.0978 - 0.106	0.0576 - 0.0624	0.0264 - 0.0286
H2O	Antigorite	0.12 - 0.13	_	_	_	_
H2O	Chrysotile	0.12 - 0.13	_	_	_	_
H_2O	Cronstedtite	0.13 - 0.18	0.0761 - 0.1053	0	0	0.0741 - 0.103
H_2O	Vermiculite	0.09 - 0.1	0	0	0.0081 - 0.009	0
Sx (but mostly S2 until about 900 K where x>2 play more significant role	Pyrite	0.53	0	0	0.0345	0.0133
Sx (but mostly S2 until about 900 K where x>2 play more significant role	Pyrrhotite (FeSx), assuming x = 1.14, (Harries+, 2013)	0.4	0.0116	0.018	0	0
H_2O	Epsomite	0.56	0	0	0.0336	0
H_2O	Smectite	0.026 - 0.04	0	0	0.0013 - 0.002	0
CO_2	Calcite	0.44	0.00484	0	0	0.0044
H_20	Sub-butiminous Coal	0.296	0	0	0.0148	0.0104
CO_2	Sub-butiminous Coal	0.149	0	0	0.00745	0.005
CO	Sub-butiminous Coal	0.074	0	0	0.0037	0.0026
CH_4	Sub-butiminous Coal	–	0	0	–	–
CO_2	Isolated Kerogen	0.65	0.0228	0.0325	0	0
CO	Isolated Kerogen	_	_	_	0	0
CH_4	Isolated Kerogen	_	_	_	0	0

Assumptions Made Regarding Volatile Release Chemistry Based on Literature Review

Event	Chemical Reaction	Released Gas	Temperature Range (ºC)	Source Mineral	Enthalpy of Reaction	Citation
Vaporization of free H2O	**Dehydration**	H_2O	30°-50° C	Atmospherically adsorbed, Preparation process water	–	1.
Vaporization of clay-bound fluids	**Dehydration**	H_2O	65°-150° C	Smectite	110 KJ/Kg	2.
Vaporization of clay-bound fluids	**Dehydration**	H2O	65°-150° C	Vermiculite	504.19 g/mol	–
Decomposition of Mg-serpentine	**Dehydroxylation**	H_2O	550 - 700	Lizardite	Lizardite 565 kJ/kg	3.
Decomposition of Mg-serpentine	**Dehydroxylation**	H2O	650 - 800	Antigorite	Antigorite 367 kJ/kg	4.
Decomposition of Mg-serpentine	**Dehydroxylation**	H2O	550 - 700	Chrysotile	Chrysotile 414 kJ/kg	4.
Decomposition of Fe-serpentine	**Dehydroxylation**	H_2O	350 - 590	Cronstedtite	–	–
Decomposition of Vermiculite	**Dehydroxylation**	H_2O	450-850	Vermiculite	68 kJ/mol	5.
Decomposition of Pyrite	**Desulphurization**	Sx (but mostly S2 until about 900 K where x>2 play more significant role	250 - 740	Pyrite	290.4 KJ/Kg	6.
Decomposition of Pyrrohotite	**Desulphurization**	Sx (but mostly S2 until about 900 K where x>2 play more significant role	250 - 740	Pyrrhotite (FeSx), assuming x = 1.14, (Harries+, 2013)	285 kJ/mol of S2 (For S2 formation 600-900K, from the reaction FeS2 -> FeSx), futher FeS -> Fe + 0.5S2 has 166 kJ/mol of FeS at 298 K)	7.
Decomposition of Epsomite	**Dehydration**	H_2O	25-275	Epsomite	351.4 kJ/mol	8.
Decomposition of smectite	**Dehydroxylation**	H_2O	700° -800° C	Smectite	320 KJ/Kg	9.
Decomposition of calcite	**Decarbonation**	CO_2	600°-850° C	Calcite	178 kJ/mol	10.
Coal decomposition	**Pyrolysis**	H_20	300 - 800	Sub-butiminous Coal	120 KJ/Kg	11.
Coal decomposition	**Pyrolysis**	CO_2	300 - 800	Sub-butiminous Coal	120 KJ/Kg	11.
Coal decomposition	**Pyrolysis**	CO	300 - 800	Sub-butiminous Coal	120 KJ/Kg	11.
Coal decomposition	**Pyrolysis**	CH_4	300 - 800	Sub-butiminous Coal	120 KJ/Kg	11.
Kerogen and bitumen pyrolysis	**Pyrolysis**	CO_2	>350° C	Isolated Kerogen	360 KJ/Kg	12.
Kerogen and bitumen pyrolysis	**Pyrolysis**	CO	>350° C	Isolated Kerogen	360 KJ/Kg	12.
Kerogen and bitumen pyrolysis	**Pyrolysis**	CH_4	>350° C	Isolated Kerogen	360 KJ/Kg	12.

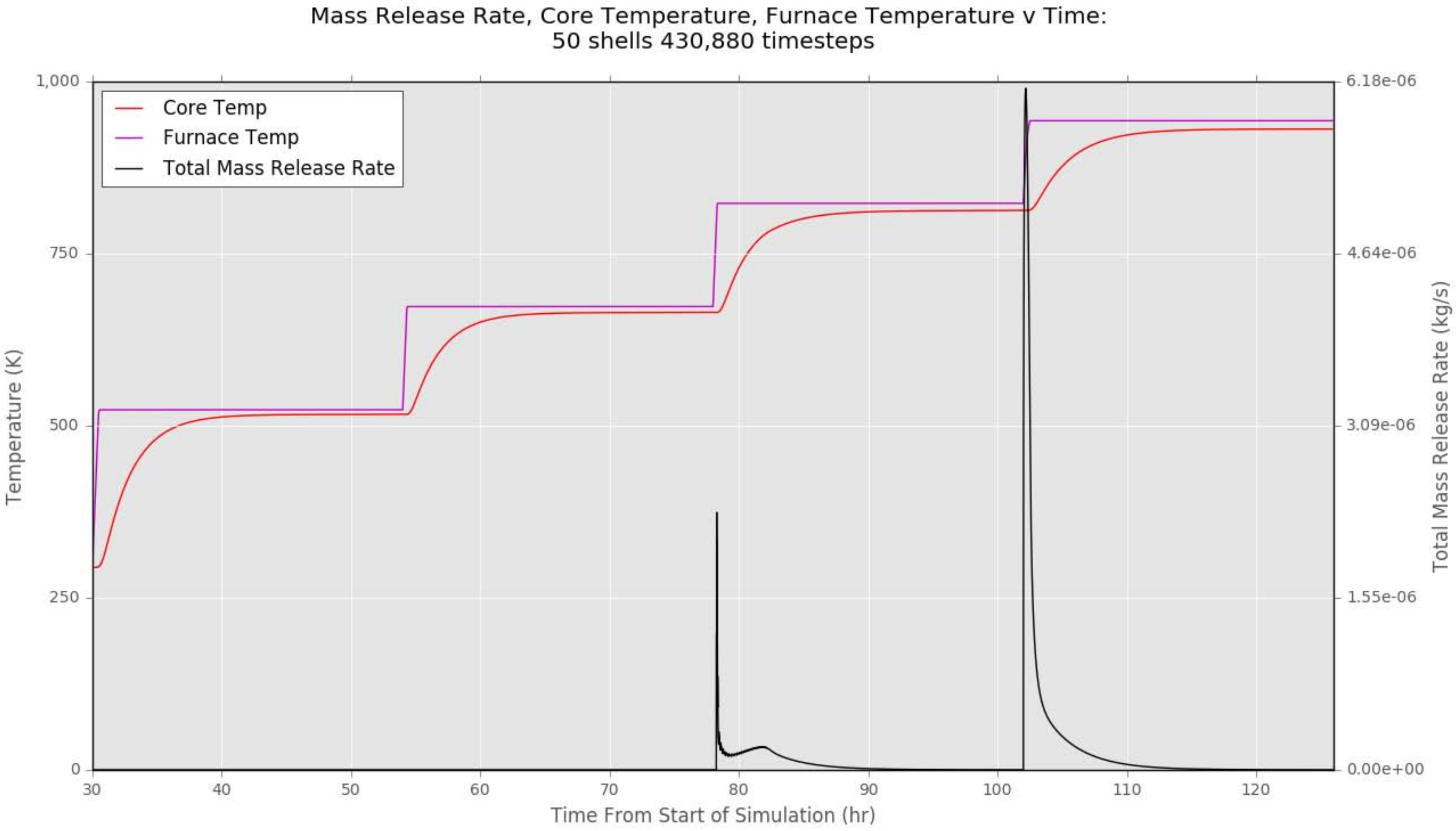
Citations for Chemistry Assumptions

1. ESI Experiments (2016)
2. Hamada et al (2009)
3. Dlugogorski+, 2014, Weber+, 1965
4. Dlugogorski+, 2014
5. Ogorodova+-2012
6. Adam J. Berkovich, John H. Levyb, S. James Schmidtc, Brent R. Young (2000)
7. Hu+, 2006
8. van Essen+, 2009
9. Hamada et al (2009)
10. Rodriguez-Navarro, 2009
11. Jerzy Tomeczek, Henry Palugniok (1996)
12. Adam J. Berkovicha, John H. Levyb, S. James Schmidtc, Brent R. Young (2000)

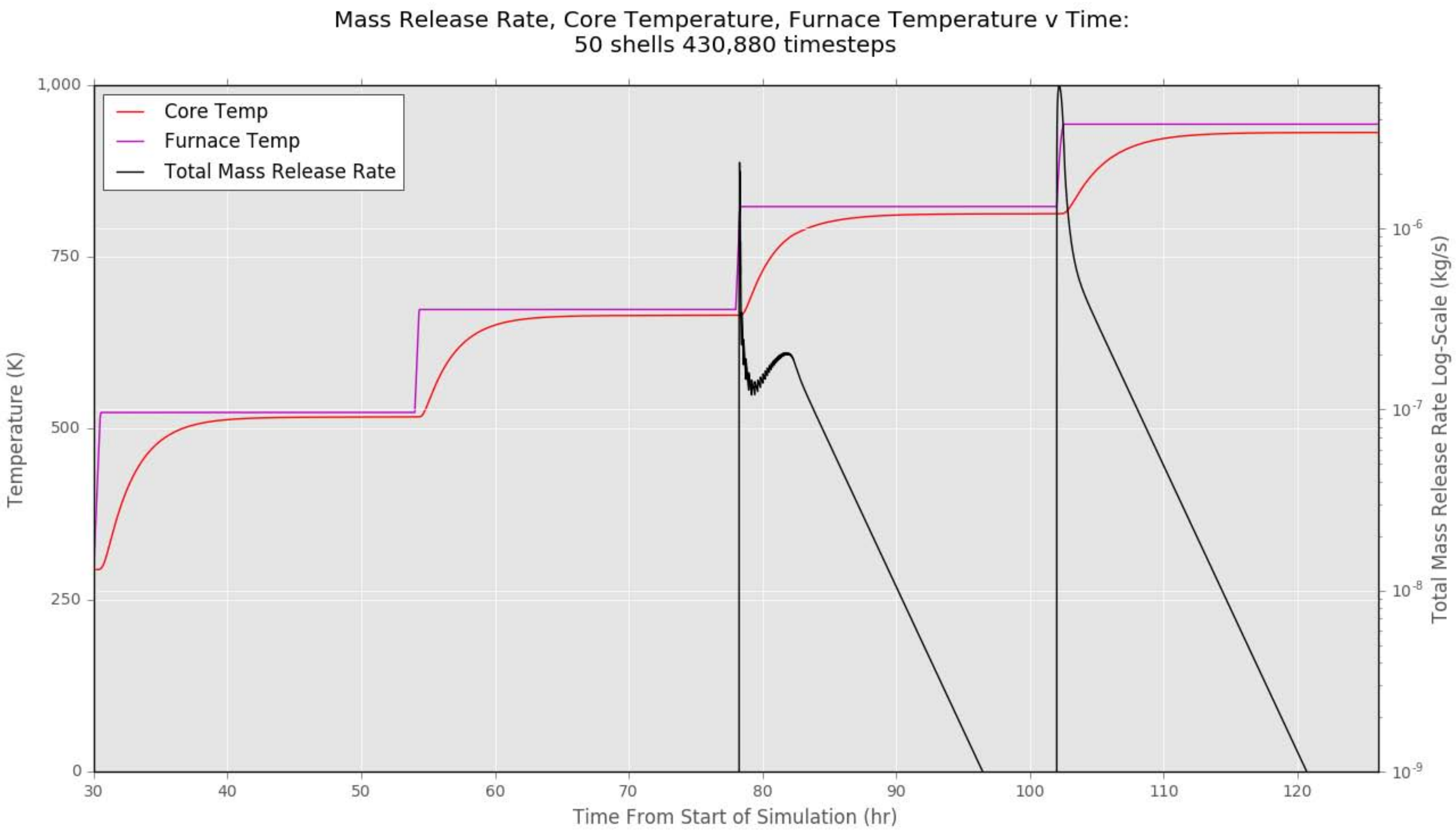
Example Model Inputs for Granular Serpentine Simulation

Granular Serpentine	
Number of Plateaus	4
Sample Thermal Time Constant (s)	20,052
Sample Mass A Priori (kg)	0.501
Thermal Conductivity	0.100
Specific Heat	800
Mineral 1	Serpentine
Mass Fraction	1
Gas 1	H2O

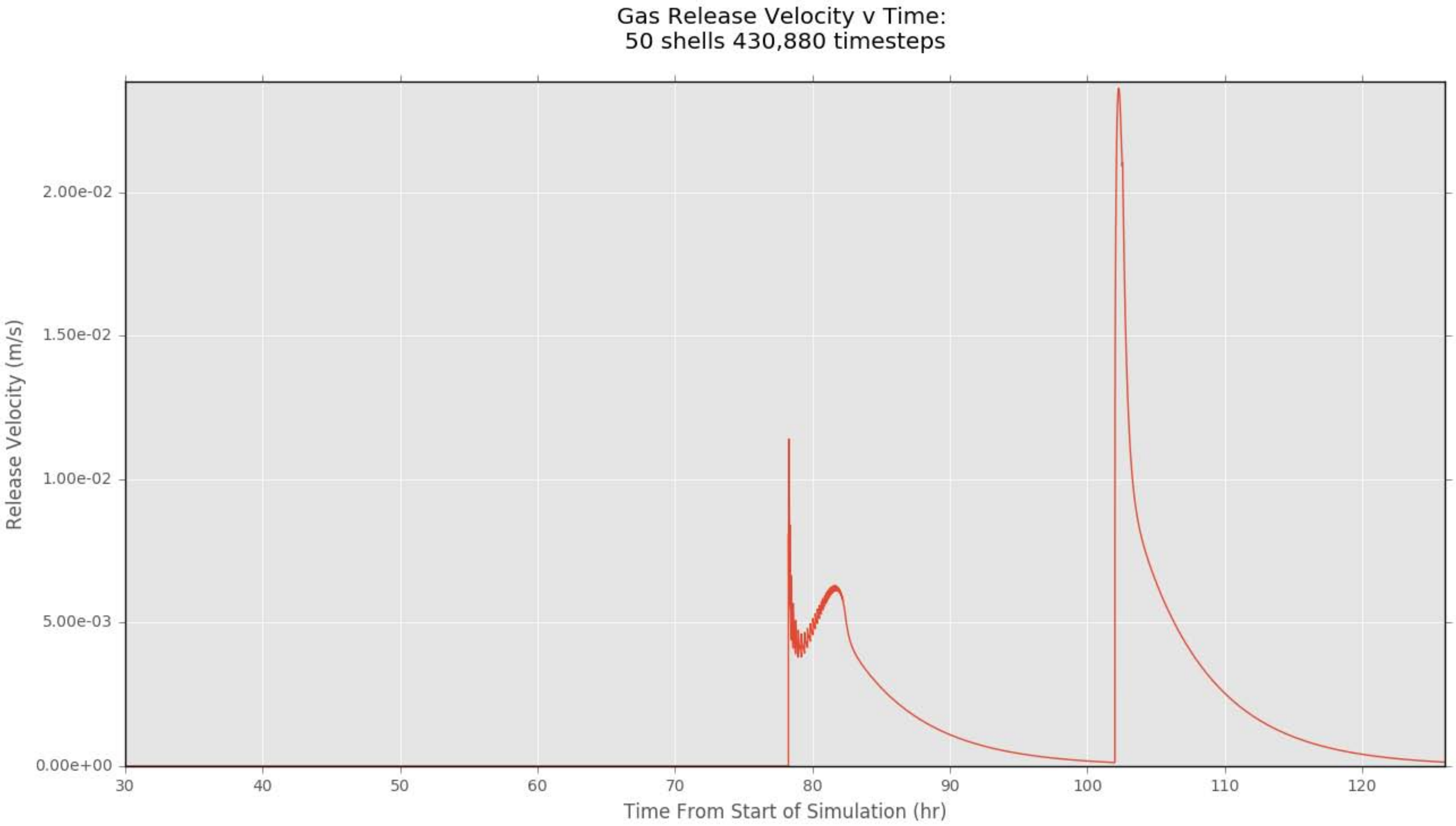
Example Result:
Granular Serpentine



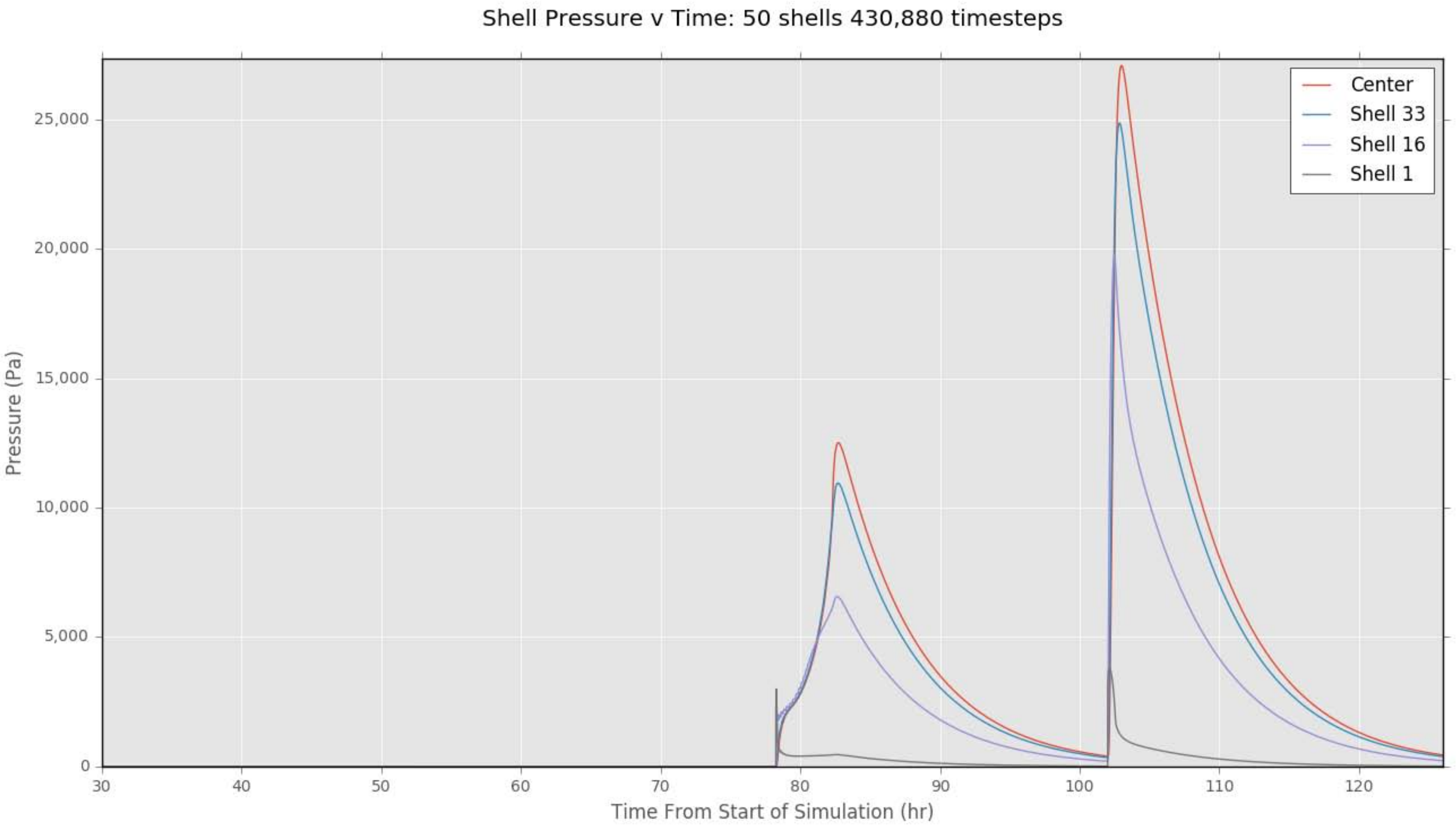
Example Result:
Granular Serpentine



Example Result:
Granular Serpentine



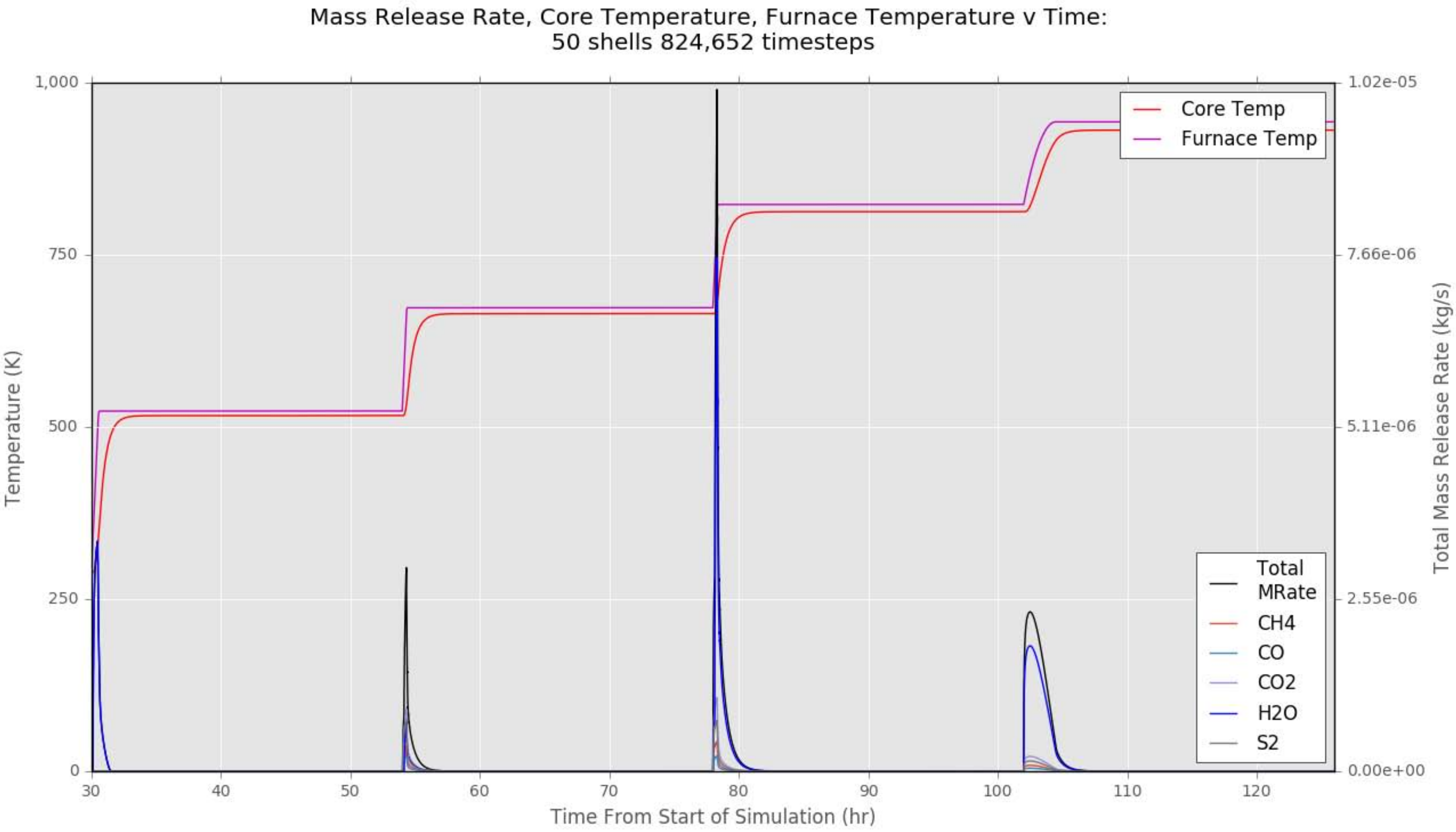
Example Result: Granular Serpentine Internal Gas Pressure Based on Darcian Diffusion



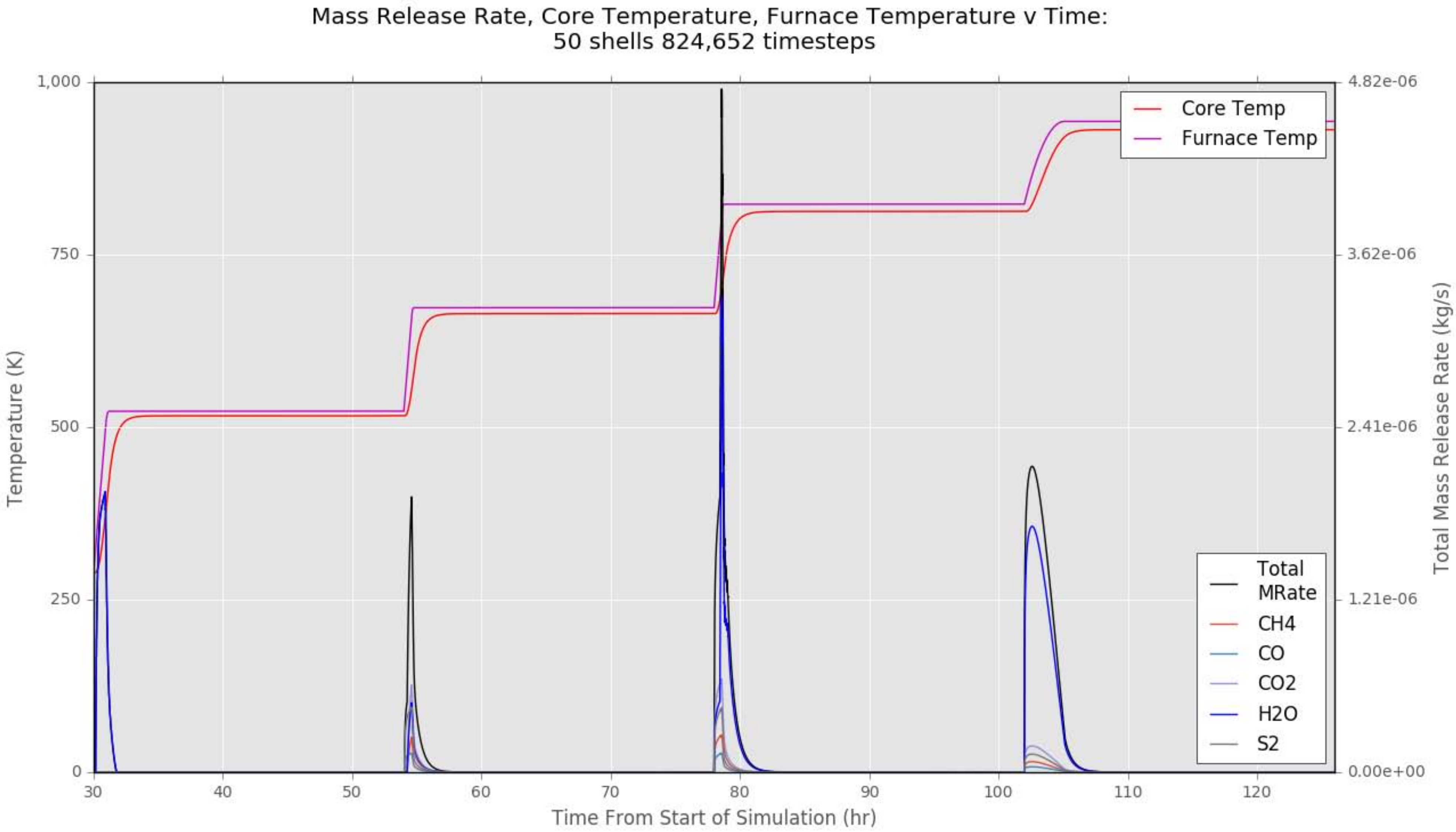
Example Model Inputs for CI Simulant Type Brick Simulation

CLASS 3 Brick Test	
Number of Plateaus	4
Sample Thermal Time Constant (s)	4,463
Sample Mass A Priori (kg)	0.488
Thermal Conductivity	0.500
Specific Heat	800
Mineral 1	Serpentine
Mass Fraction	0.48
Mineral 2	Sub-Bituminous Coal
Mass Fraction	0.05
Mineral 3	Pyrite
Mass Fraction	0.065
Gas 1	H_2O
Gas 2	CO_2
Gas 3	CH_4
Gas 4	CO
Gas 5	S_2

CI Simulant Brick, Oven Temperature Ramp Rate as Observed in Experiment

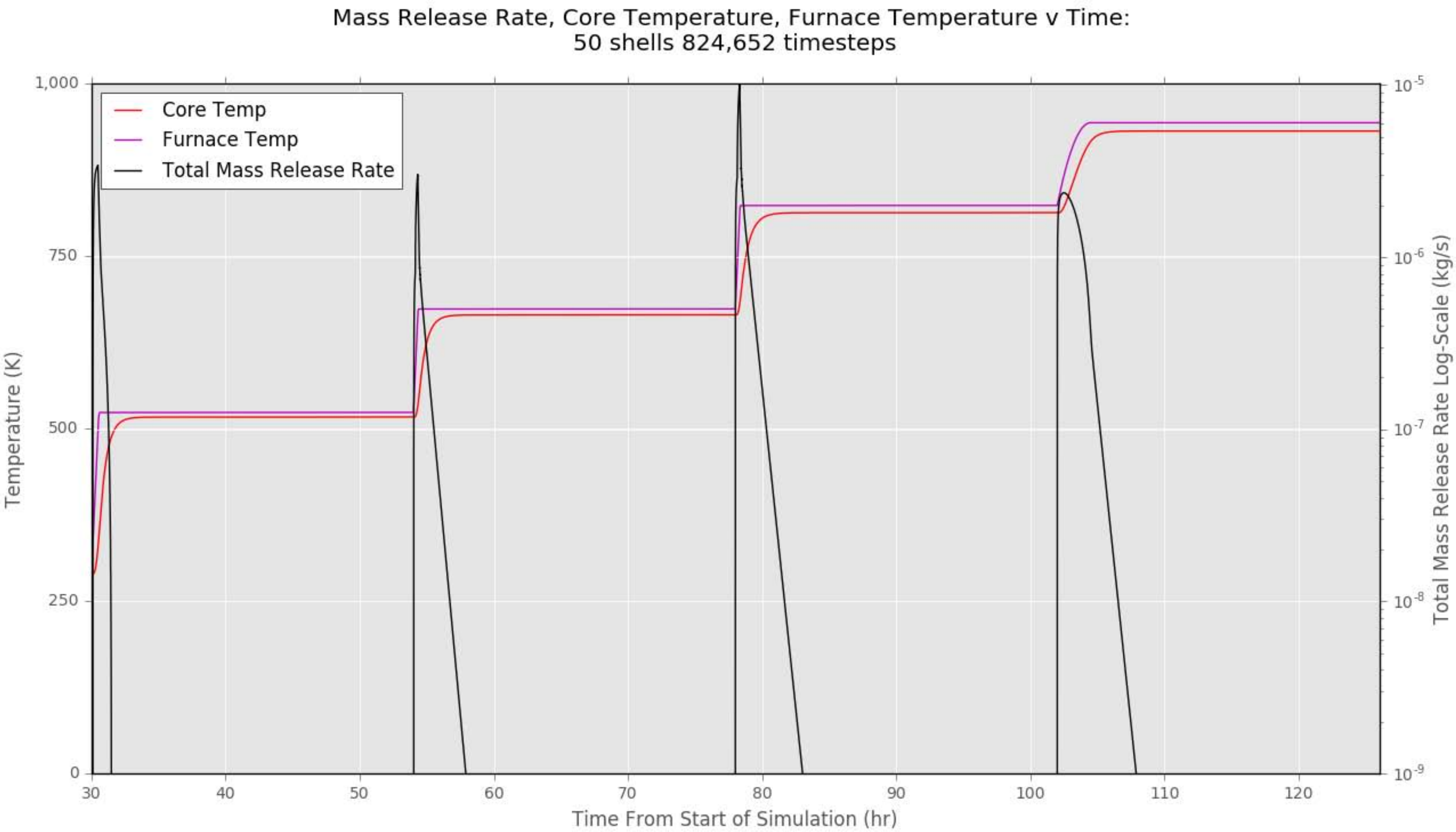


CI Simulant Brick, ~50% Observed Oven Temperature Ramp Rate

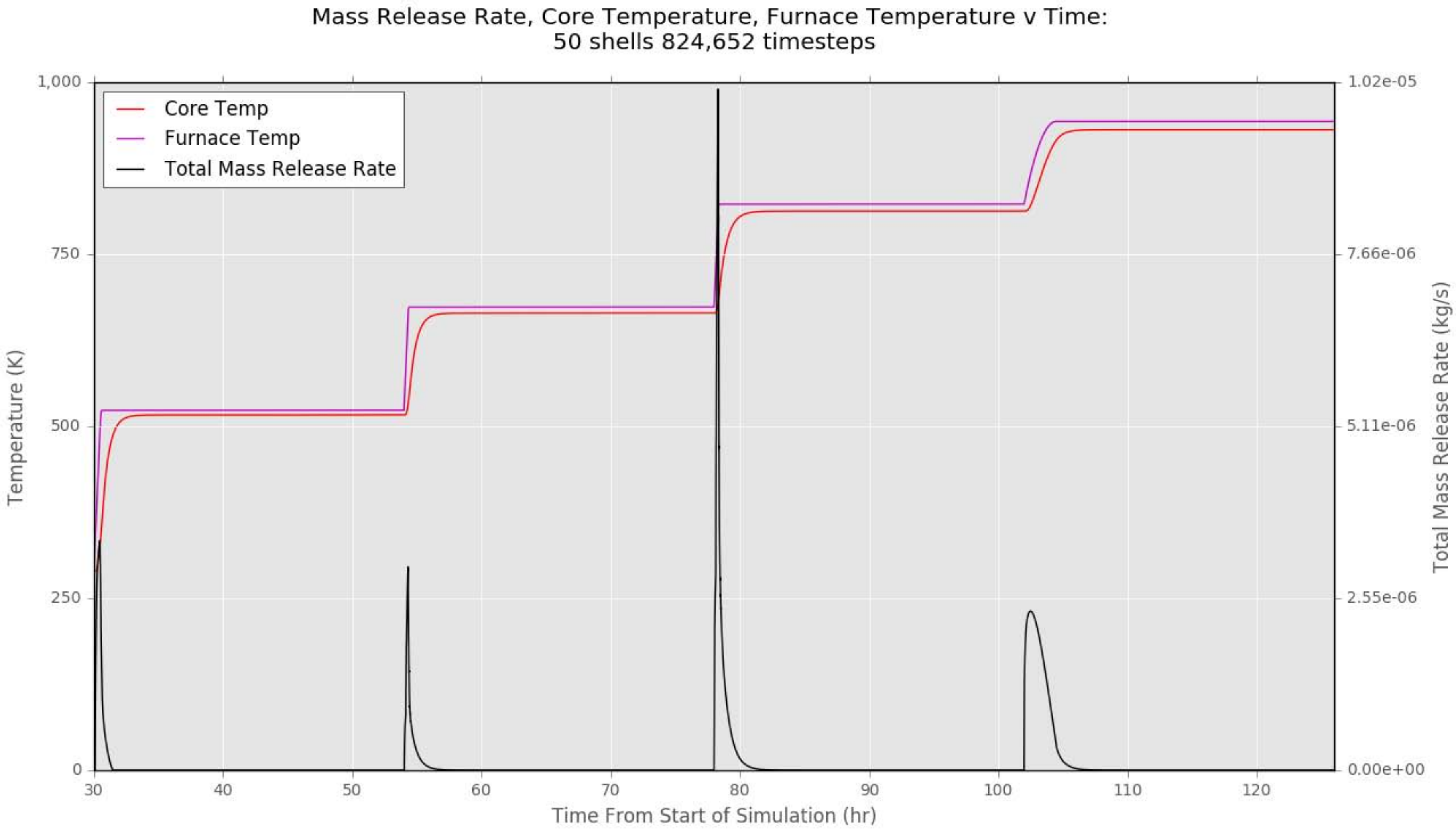


Excellent Agreement With Experiment!

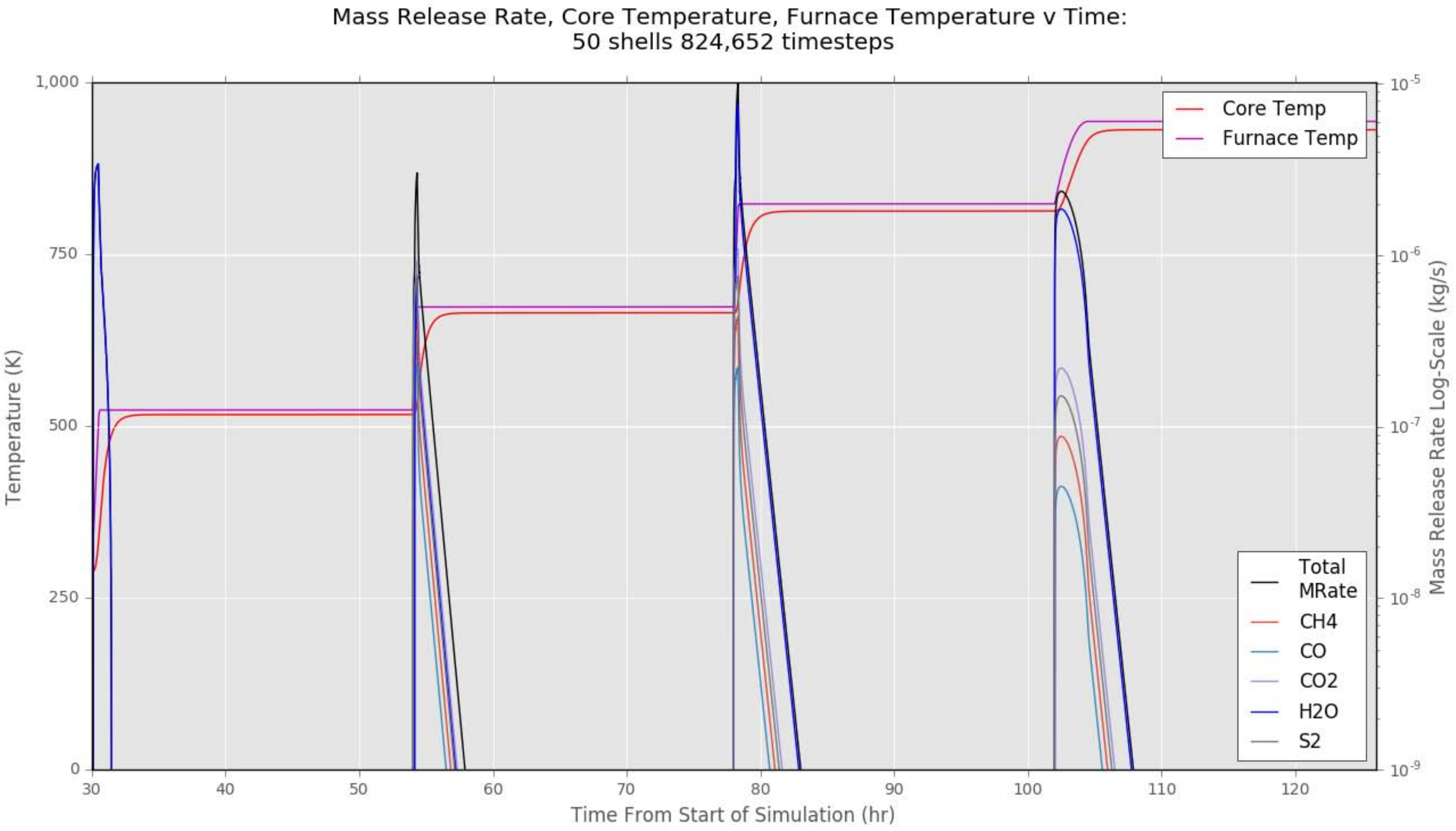
Example Result: CI Simulant Type Brick Simulation



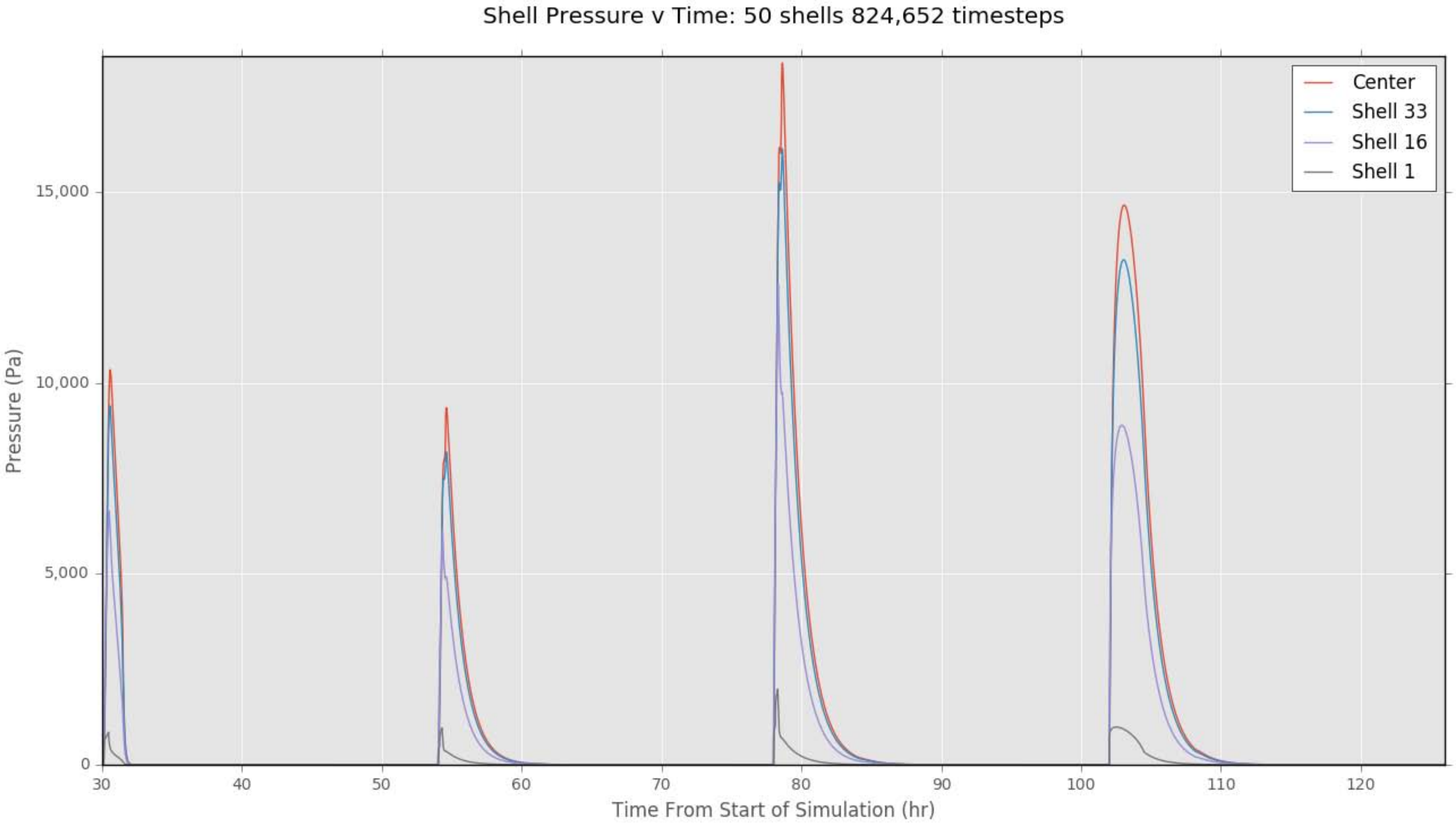
Example Result: CI Simulant Type Brick Simulation



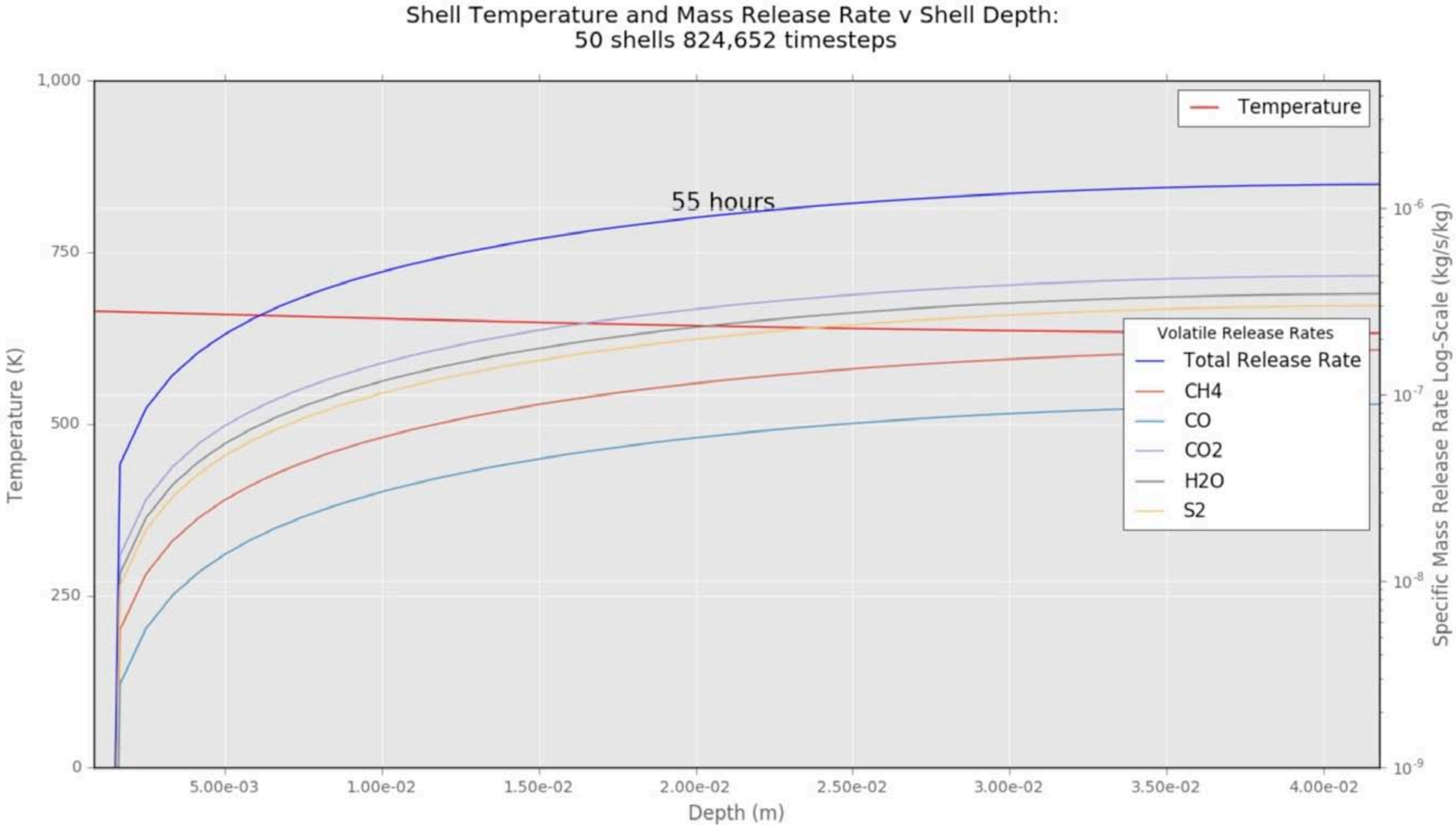
Example Result: CI Simulant Type Brick Simulation



Example Result: CI Simulant Type Brick Simulation: Internal Gas Pressure



Example Result: CI Simulant Type Brick Simulation



Screen Grab of Time Sequence Animation

CI Simulant Brick Simulation Results

Analysis of Simulation Data, Total Mass Release

	Plateau		Mass in grams		
Plateau Temp:	250 deg C	400 deg C	550 deg C	645 deg C	
CH4	0.00	0.45	0.72	0.58	
H2O	5.94	1.11	9.83	12.25	
CO/N2	0.00	0.35	0.37	0.30	
CO2	0.00	0.89	1.81	1.45	
S2/SO2	0.00	1.19	1.25	1.00	
Total	**5.94**	**3.99**	**13.97**	**15.56**	**39.47**

CI Simulant Brick Simulation Results

Analysis of Simulation Data, Mass Fractions

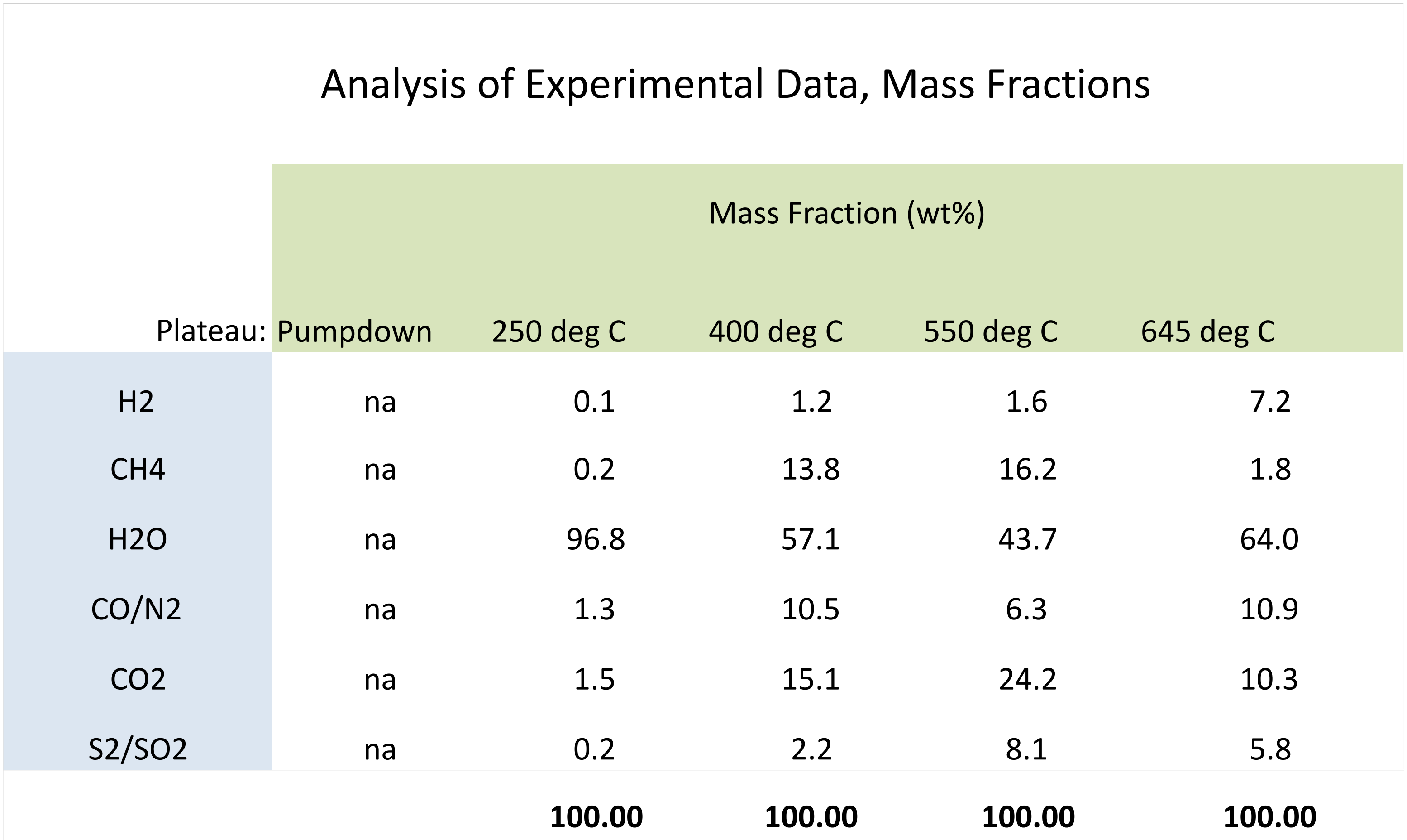
	Mass Fraction (wt%)			
Plateau Temp:	250 deg C	400 deg C	550 deg C	645 deg C
CH4	0.0	11.2	5.2	3.7
H2O	100.0	27.9	70.3	78.7
CO/N2	0.0	8.8	2.6	1.9
CO2	0.0	22.3	12.9	9.3
S2/SO2	0.0	29.8	8.9	6.4
	100.00	**100.00**	**100.00**	**100.00**

CI Simulant Brick Experimental Results

Analysis of Experimental Data, Integrated Mass Release Rate

	Mass in grams					
Plateau Temp:	Pump	250 deg C	400 deg C	550 deg C	645 deg C	
H_2	na	0.00	0.04	0.24	1.13	
CH_4	na	0.01	0.41	2.52	0.29	
H_2O	na	6.00	1.69	6.81	10.09	
CO/N_2	na	0.08	0.31	0.99	1.72	
CO_2	na	0.09	0.45	3.78	1.62	
S_2/SO_2	na	0.01	0.06	1.25	0.91	
Total		**6.19**	**2.96**	**15.58**	**15.75**	**40.48**

CI Simulant Brick Experimental Results



Analysis of Experimental Data, Mass Fractions

	Mass Fraction (wt%)				
Plateau:	Pumpdown	250 deg C	400 deg C	550 deg C	645 deg C
H2	na	0.1	1.2	1.6	7.2
CH4	na	0.2	13.8	16.2	1.8
H2O	na	96.8	57.1	43.7	64.0
CO/N2	na	1.3	10.5	6.3	10.9
CO2	na	1.5	15.1	24.2	10.3
S2/SO2	na	0.2	2.2	8.1	5.8
		100.00	**100.00**	**100.00**	**100.00**

CI Simulant Brick Experimental Results

Mass Measured on the cyrotrap

Mass in grams

	Pumpdown	250 deg C	400 deg C	550 deg C	645 deg C	Total
Actual Ice	19.7	11.5	4.4	11.8	20.8	**48.5**
Actual Liquid	19.6	10.9	3.3	11.2	17.2	**42.6**
Difference	0.1	0.6	1.1	0.6	3.6	**5.9**

Comparison to Experimental Analysis

		250 deg C	400 deg C	550 deg C	645 deg C	Total
Likely Ice (H2O+CO2)		6.1	2.1	10.6	11.7	**30.5**
Likely Liquid (H2O)		6.0	1.7	6.8	10.1	**24.6**
Difference (CO2)		0.1	0.4	3.8	1.6	**5.9**

Summary Comparison of Model with Experiment

- Time dependent thermal response within 2X
  - Primary difference is that gas release rates in the model are higher and occur over a shorter period than as measured
  - The difference goes away when oven ramp rate is cut by 2X
  - This may be a facility instrumentation issue related to the thermal time constant of the oven v.s. the thermal response of thermocouples close to heater units
- Excellent qualitative agreement.
- Total yield agreement within 2 percent.
- Agreement on water yield within 16 percent for hydrates.
- Mix of carbon based yields will require additional model tuning, specifically with regards to chemistry assumptions for pyrolysis; may also improve prediction for water yield.

Conclusions

- Internal gas pressure is moderate and gas diffusion times are negligible due to the physics of asteroid porosity
- We understand the basic physics, chemistry, and gas dynamics of the process
- Additional details are required to tune the model

Next Steps..

- Model tuning
  - Mostly focussed on carbon chemistry pyrolysis
- Detailed comparison with experiment and publication of more complete results
- Extension of model to embrace Optical Mining™