A Simple High Temperature Battery Model

or Basic Gas and Solid Heat Balance for a High Temperature Thermal Battery

As a Python practice exercise, I coded up what I think is a full featured model for a high temperature thermal battery. Before I did the actual coding, I derived the equations for a simplified model to get some insight into the battery physics. I model the battery as a packed bed where the solid stores heat at high temperature and a working fluid extracts heat from the solid and delivers it to a target. I imagine CO2 as the working fluid because it can radiatively participate in the heat transfer which should work to our advantage when extracting and delivering heat.

I wrote this article because I think this kind of analysis is a useful first step when modeling systems of all kinds. I learned some helpful lessons from this exercise. I hope it is a usefull example for the reader.

A rough outline of my approach is as follows:

- Derive the gas side balance including radiative exchange between solid and a radiatively participating gas that I assume to be CO2
- Derive the solid side balance including radiative heat transfer through the bed.
- Identify the dimensionsless numbers that govern the system and describe their physical meaning.
- Generate an order of magnitude estimate for the dimensionless numbers using nominal or average physical proprties and assess their relative importance.

It is important to identify the simplifying assumptions:

- I assume the battery is isobaric, so I don't solve for pressure drop
- I assume all physical properties are constant at nominal or average values

Of course, a rigorous analysis is required to move from simplified system to full featured model. But that is another article for another day.

A Thousand Words

Before diving into math, we need to think about the physical phenomena we want our model to capture. Figure 1 is a cartoon that illustrates how I think about the battery physics and I will list the important phenomena here:

- Plug flow of gas through a packed bed of hot solids
- Convective transfer of heat from the packed bed solids to the gas
- Radiative transfer of heat from the packed bed solids to the radiatively participating gas
- Conduction of heat axially through the bed
- Radiative transfer of heat axially through the bed.

All leading to an exiting flow of high temperature gas we send away to heat the target before it eventually cirdulates back to the bed as a cool gas to be heated again.

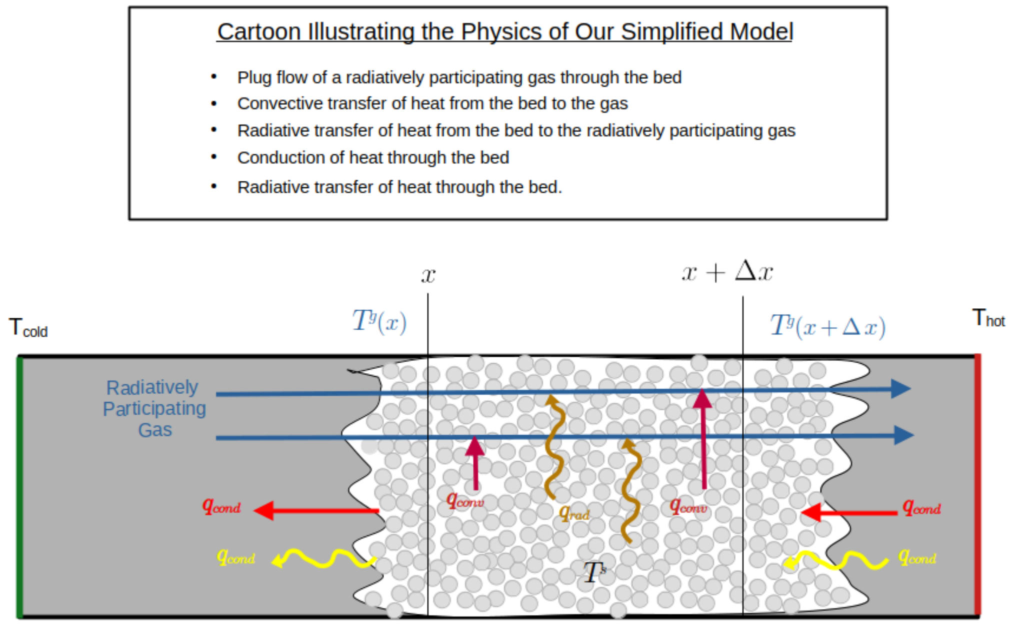

Figure 1: *Cartoon illustrating the physics we want to capture in our simplified model.*

In the next couple of sections I develop the math corresponding to Figure 1.

Gas Balance

All of the parameters that I will use in this derivation are described in the Nomenclature section at the end of this article. I will only define a few key parameters as they are introduced. But I direct the reader to Table 1 if any of the nomenclature is unclear.

The shell balance for a differential volume of gas is

$$\dot{m}C_p^g(T\big|_{x+dx} - T\big|_x) = C_a \Delta x S_a h * (T_s - T_g) + C_a \Delta X S_a (\sigma\epsilon)_{g.s}(T_s^4 - T_g^4)$$

where S_a is the bed specific surface area, h is the convective heat transfer coefficient and $(\sigma\epsilon)_{g.s}$ quantifies radiative heat transfer between gas and solid.

Dividing by Δx and taking the limit

$$\dot{m}C_p^g \frac{\partial T_g}{p\partial x} = C_a S_a[h(T_s - T_g) + (\sigma\epsilon)_{g.s}(T_s^4 - T_g^4)]$$

And I next define the following dimenstionless variables

$$x^* = \frac{x}{L} \qquad T^* = \frac{T}{T_{max}}$$

and let

$$\sigma^*_{g.s} = (\sigma\epsilon)_{g.s}$$

then

$$\frac{\dot{m}C_p^g T_{max}}{C_a L S_a}\frac{\partial T_g^*}{\partial x^*} = hT_{max}(T_s^* - T_g^*) \;+\; \sigma^*_{g.s}T_{max}^4({T_s^*}^4 - {T_g^*}^4)$$

which I can rearrange to be

$$\frac{\partial T_g^*}{\partial x^*} = \frac{S_{tot}h}{\dot{m}C_p^g}(T_s^* - T_g^*) \;+\; \frac{S_{tot}\sigma^*_{g.s}T_{max}^3}{\dot{m}C_p^g}({T_s^*}^4 - {T_g^*}^4)$$

and I let $C_a L S_a = S_{tot}$,the total surface area in the bed,

I define $\sigma^*_{g.s}$ as the modified Stefan-Boltzmann constant that characterizes the efficiency of solid-to-gas radiative heat transfer. It is a function of emissivity on the solid side and effective emissivity on the gas side. The gas side effective emissivity is a function of the gas composition and pressure and the average pathlength for adsorbtion.

If the working fluid is a radiatively **non**-participating gas, like air, then the radiative term will disappear and heat will transfer only by convection. Obviously, I'm hoping that by using a radiatively participating gass, I can accelerate gas heating by augmenting convection with radiation.

This equation tells us that the rate of temperature change of a differential volume of gas flowing across a differential volume of bed is determined by the heat transfered from solid to gas by convection plus the heat transfered from solid to gas by radiation.

Solid Balance

The shell balance for a differential volume of solid is

$$C_a\Delta X\rho_{bed}C_p^s\frac{\partial T_s}{\partial t} = -\dot{m}C_p^g\left[T_g\Big|_{x+\delta x} - T_g\Big|_x\right] + C_a k_{eff}\left[\frac{\partial T_s}{\partial x}\Big|_{x+\delta x} - \frac{\partial T_s}{\partial x}\Big|_x\right] + C_a\sigma^*\delta\left[\frac{\partial T_s^4}{\partial x}\Big|_{x+\delta x} - \frac{\partial T_s^4}{\partial x}\Big|_x\right]$$

And I am using the constitutive equation for radiative flux derived in my article titled Hot Plates

$$q_{rad} = \sigma^*\delta\frac{\partial T^4}{\partial x}$$

and δ is the length between theoretical radiative plates. I had approximated $\delta = 4d_p$ for a packed bed of spheres, but for right now, I will leave it as δ, to be approximated later.

Pressing on, I divide by Δx and take the limit

$$C_a \rho_{bed} C_p^s \frac{\partial T_s}{\partial t} = -\dot{m} C_p^g \frac{\partial T_g}{\partial x} + C_a k_{eff} \frac{\partial^2 T_s}{\partial x^2} + C_a \sigma^* \delta \frac{\partial^2 T_s^4}{\partial x^2}$$

I will add dimensionless time to the dimensionless variables used previously.

$$x^* = \frac{x}{L} \qquad T^* = \frac{T}{T_{max}} \qquad t^* = \frac{\dot{m} t}{M}$$

then

$$\frac{C_a \rho_{bed} C_p^s T_{max} \dot{m}}{M} \frac{\partial T_s^*}{\partial t^*} = -\frac{\dot{m} C_p^g T_{max}}{L} \frac{\partial T_g^*}{\partial x^*} + \frac{C_a k_{eff} T_{max}}{L^2} \frac{\partial^2 T_s^*}{\partial x^{*2}} + \frac{C_a \sigma^* \delta T_{max}^4}{L^2} \frac{\partial^2 {T_s^*}^4}{\partial x^{*2}}$$

sparing the reader all the algebra, by rearranging and canceling terms I get

$$\frac{\partial T_s^*}{\partial t^*} = -\frac{C_p^g}{C_p^s} \frac{\partial T_g^*}{\partial x^*} + \frac{k_{eff}}{L C_p^s G} \frac{\partial^2 T_s^*}{\partial x^{*2}} + \frac{\sigma^* T_{max}^3 \delta}{L C_p^g G} \frac{\partial^2 {T_s^*}^4}{\partial x^{*2}}$$

and I've taken advantage of the following

$$C_a L \rho_b = M \qquad \frac{\dot{m}}{C_a} = G$$

where G is the mass flux and M is the total mass of solid in the bed .

This equation tells us that the rate of change of the solid temperature in a differential bed volume depends on the amount of heat transfered to the gas and the heat that is transferred axially into or out of the volume by conduction or by radiation.

Figure 2 shows the cartoon of our bed, but this time the bullet points describing the physics have been replaced by the model equations. Now would be a good time for the reader to make sure that the connections from cartoon to bullet point to terms in the equation is clear for all the phenomena we are trying to capture.

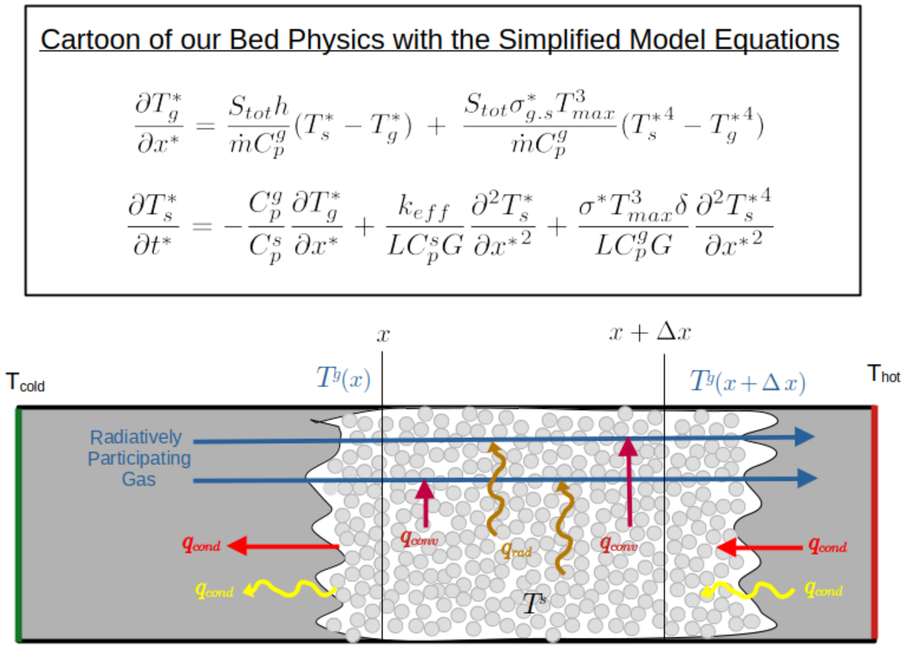

Figure 2: *Cartoon of the bed with our simplified model equations.*

The Dimensionless Numbers

Lets rewrite the dimensionless forms of the gas and solid heat balances and then extract the governing dimensionless numbers.

The dimensionless gas balance

$$\frac{\partial T_g^*}{\partial x^*} = \frac{S_{tot}h}{\dot{m}C_p^g}(T_s^* - T_g^*) + \frac{S_{tot}\sigma_{g.s}^* T_{max}^3}{\dot{m}C_p^g}({T_s^*}^4 - {T_g^*}^4)$$

The dimensionless solid balance

$$\frac{\partial T_s^*}{\partial t^*} = -\frac{C_p^g}{C_p^s}\frac{\partial T_g^*}{\partial x^*} + \frac{k_{eff}}{LC_p^s G}\frac{\partial^2 T_s^*}{\partial {x^*}^2} + \frac{\sigma^* T_{max}^3 \delta}{LC_p^g G}\frac{\partial^2 {T_s^*}^4}{\partial {x^*}^2}$$

And these equations define the following dimenstionless numbers:

$$N_{conv} = \frac{S_{tot}h}{\dot{m}C_p^g}$$

$$N_{g.s.rad} = \frac{S_{tot}\sigma_{g.s}^* T_{max}^3}{\dot{m}C_p^g}$$

$$N_{cond} = \frac{k_{eff}}{LC_p^s G}$$

$$N_{s.s.rad} = \frac{\sigma^* T_{max}^3 \delta}{LC_p^g G}$$

$$N_{hcap} = \frac{C_p^g}{C_p^s}$$

The first, N_{conv}, is also known as NTU or the Number of Transfer Units. It is the ratio of convective heat transfer capacity to thermal carrying capacity. It is the same number used in the effectiveness-NTU method for heat transfer in packed beds. The third, N_{cond}, is the inverse Peclet number, $\frac{1}{Pe}$, and is the ratio of bed axial conduction to gas thermal carrying capacity

The second and fourth dimensionless numbers characterize radiation. $N_{g.s.rad}$, is the ratio of solid-gas radiative heat transfer capacity to thermal carrying capacity and is the radiative analog of NTU. $N_{s.s.rad}$, is the ratio of bed radiative axial heat transfer to gas thermal carrying capacity and it is the radiative analog of the inverse peclet number for conduction.

Lastly, we have the ratio of heat capacities, N_{hcap}, which relates the gas temperature gradient to the rate of change of solid temperature.

So, two equations - the gas and solid heat balances - give us five governing dimensionless quantities, that can teach us a lot. For example, to maximize the rate of gas heating we want to maximize N_{conv} and $N_{g.s.rad}$, and we might maximize the ratio of $\frac{S_{tot}}{\dot{m}}$. To minimize axial heat transfer, we want to minimize N_{cond} and $N_{s.s.rad}$, and could aim for a high aspect ratio (a large L for a given bed volume), or design to minimize δ, the distance beteen radiative plates.

In the next section I'll ballpark a design (a slightly-educated guess at the pysical dimensions of a commercial high temperature battery). Then I'll estimate the remaining paraneters to arrive at order of magnitude estimates for our dimensionless numbers.

A Ballpark Design

Figure 3 is a cartoon of a high temperature thermal battery implementation. The working fluid, CO2, is heated as it moves through the bed and then hot CO2 delivers heat to the target by a combination of radiation and convection. After delivering its heat, the cool CO2 is circulated back through the bed to be heated again. As the gas extracts heat from the bed, the bed temperature drops. The trick is to create a bed temperature profile that allows most of the heat to be extracted before the outlet temperature begins to fall.

We want our ballpark design to be at a commercially relevant scale. I'll assume that we need 10 hours of storage for a system delivering 150 MW of heat so my battery has to store 1.5 GW-hrs heat. I will further assume the following:

- Inlet gas temperature is 400 K, which is the minimum battery temperature, T_{min}
- Heat is stored at 2000 k, which is the maximum battery temperature, T_{max}.
- My battery consists of two separate beds with square cross section
- Each bed has an aspect ratio of 4 so that $H = 4L$ for each bed
- The bed porosity is 0.4

- The heat capacity of the solid, C_p^s is $1270 \frac{J}{kgK}$
- The heat capacity of our working fluid, CO_2 is $1200 \frac{J}{kgK}$
- The solid density, ρ_s, is $2400 \frac{kg}{m^3}$
- The density of the bed is $\rho_s(1-\epsilon)$, or $1440 \frac{kg}{m^3}$
- The required total heat storage, Q is 1.5 $GW - hrs$
- The required total heat delivery, q_{tot}, is $150 MW$

Even though I am not rigorously calculating pressure drop across the bed I've scoped the design with a low aspect ratio to keep the pressure drop small. I have also assumed we need two separate beds to minimize flow maldistribution that can occur with flow through beds with large cross sectional areas. Of course, these are all assumptions that are subject to a more rigurous analysis later.

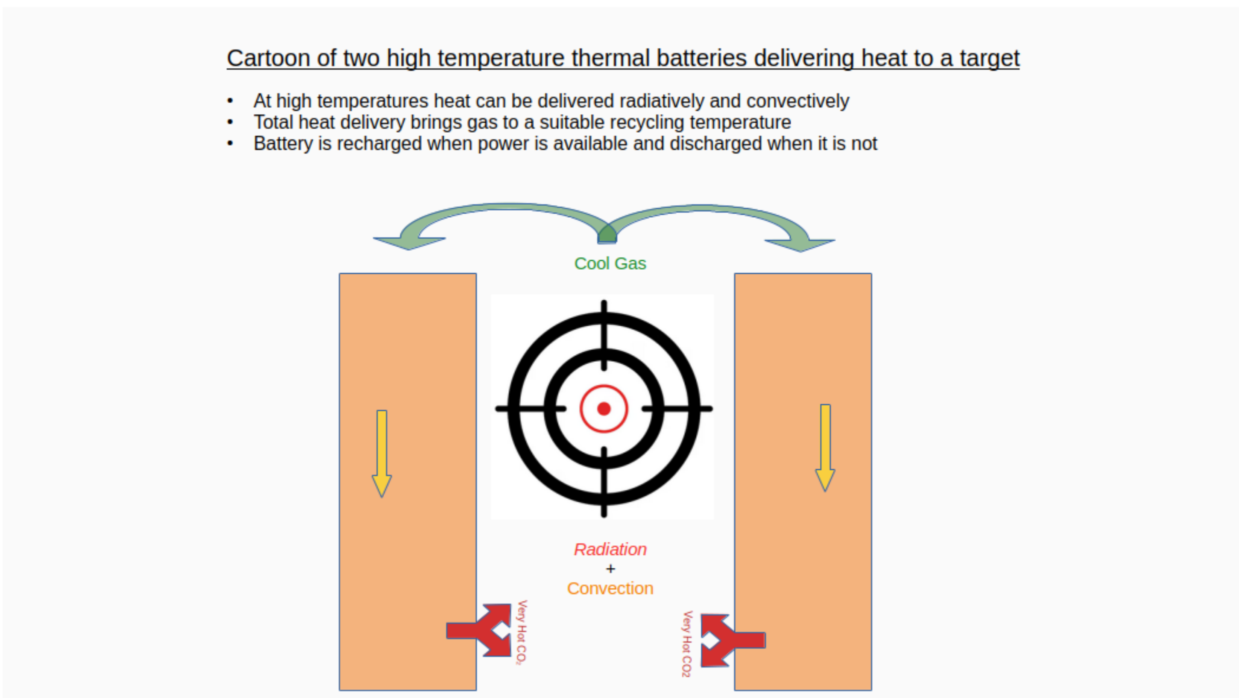

Figure 3: *Cartoon of a high temperature thermal battery delivering heat to a high temperaure industrial process via radiation and conduction.*

With the assumptions above we can start sizing our battery. The mass of each bed is:

$$M_{bed} = \frac{Q_{bed}}{C_p^s(T_{max} - T_{min})}$$

where

$$Q_{bed} = \frac{Q_{tot}}{2}$$

Doing the algebra we find that the mass of each bed is $1.33 \times 10^6\ kg$. At a bed density of $1440\frac{kg}{m^3}$, the volume for each bed is $923m^3$. At an aspect ratio of 4 for a rectangular bed

$$L = 6.13m \qquad H = 24.5$$

In similar fashion we can find the mass flow rate of our working fluid, CO_2.

$$\dot{m} = \frac{q_{bed}}{C_p^g(T_{max} - T_{min})}$$

where $q_{bed} = \frac{q_{tot}}{2}$

The mass flowrate to each bed is $39\frac{kg}{S}$

and the mass flux through a cross sectional area of $37.6m^2$ is $1.04\frac{kg}{m^2}$

Physical Properties

To find physical property values I pulled data from the internet using a combination of Google, Grok, and Claude. I had Claude calculate the convective heat transfer coefficient, the effective gas-solid emissivity, and the inlet pressure drop. I did not create a bibliography of references, but I trust the reader can easily recreate my search to hunt down the sources.

Values for all the parameters I used are listed in the Nomenclature Section at the end of this article. For these ballpark estimates I have used physical properties at 1200 K - the midpoint between 400 K and 2000 K. Eventually, a more rigorous model will have to account for pressure drop and for physical property changes with temperature and pressure (and composition, if we want to be completely general).

The dimensionless number values are at the bottom of the table and we learn that:

$$N_{conv} = 143$$

$$N_{g.s.rad} = 52$$

$$N_{cond} = 1.49 \times 10^{-4}$$

$$N_{s.s.rad} = 9.00 \times 10^{-3}$$

$$N_{hcap} = 0.95$$

The parameters that govern convective and radiative heat transfer from gas to solild are $\mathcal{O}(10^2)$-ish, the heat capacity ratio is $\mathcal{O}(1)$, the parameters for axial bed conduction and radiative heat transfer are $\mathcal{O}(10^{-4})$ and $\mathcal{O}(10^{-2})$, respectively. And that implies the following:

- Both radiative and convective modes of heat transfer from solid to gas are important.
- Axial heat transfer is not very important (of the two axial modes, radiative transfer matters more than conduction)

If these observations hold we can simplify the solid balance equation and our model becomes:

The dimensionless gas balance

$$\frac{\partial T_g^*}{\partial x^*} = \frac{S_{tot}h}{\dot{m}C_p^g}(T_s^* - T_g^*) + \frac{S_{tot}\sigma_{g.s}^* T_{max}^3}{\dot{m}C_p^g}({T_s^*}^4 - {T_g^*}^4)$$

The dimensionless solid balance

$$\frac{\partial T_s^*}{\partial t^*} = -\frac{C_p^g}{C_p^s}\frac{\partial T_g^*}{\partial x^*}$$

Neglecting axial heat transfer makes our lives easier and simplifies the model numerical methods. That alone justifies this simplified model analysis.

What It All Means

In the scoping design, I set T_{max} to 2000 K, which is near flame temperature, and T_{min} to 400 K. There are several advantages for such high temperatures and large ΔT.

- A large solid ΔT minimizes the battery size by maximizing the heat stored in each kg of solid
- A large gas ΔT minimizes gas flow rate by maximizing the heat delivered from each kg of gas.
- High temperatures are required to deliver energy to the very high temperature sinks typical of industries like cement, steel, and petrochemicals.
- High gas temperatures allow for a large driving force and high heat fluxes. this can reduce the size (and lower the capital cost) of the heat transfer apparatus.
- At the near flame temperature of 2000 K, heat can be delivered to the target both radiatively and convenctly which opens up the design space for the heat delivering apparatus.
- At near flame temperature of 2000 K, the bed can heat the gas both radiatively and convectively which helps achieve an efficient bed temperature profile.

Figure 4 illustrates the temperature profile of an efficient battery design when it is partially discharged. The front of the battery is completely discharged and the bed temperature is near T_{min}. In the middle of the battery is an active heat transfer zone where gas is being heated by hot solid. The back of the bed is still fully charged and the temperature is near T_{max}. As the battery is discharged, this temperature profile moves through the bed until it reaches the end, at which point the outlet temperature begins to drop.

The size of the active heat transfer zone tells us the achievable battery efficiency because the heat in that zone can only be partially extracted without lowering the outlet temperature. A steep temperature profile implies a narrow heat transfer zone and we can extract most of the heat before the outlet temperature drops. I hope it is easy for the reader to see that, conversely, a wide heat transfer zone implies that we can't extract as much heat before the outlet temperature drops.

It is interesting to note that to the outside world, an efficient battery delivers heat at constant temperature as if it were latent heat. In that sense, it mimics steam heating, with which engineers are very familiar, but at much higher temperatures.

To achieve the steep temperature of an efficient battery we want: ' - Heat transfer from solid to gas to be fast and it is to our advantage that radiation can augment convective heating.

- We want axial heat transfer to be small, and our simplified analysis suggests we can design for this to be the case.

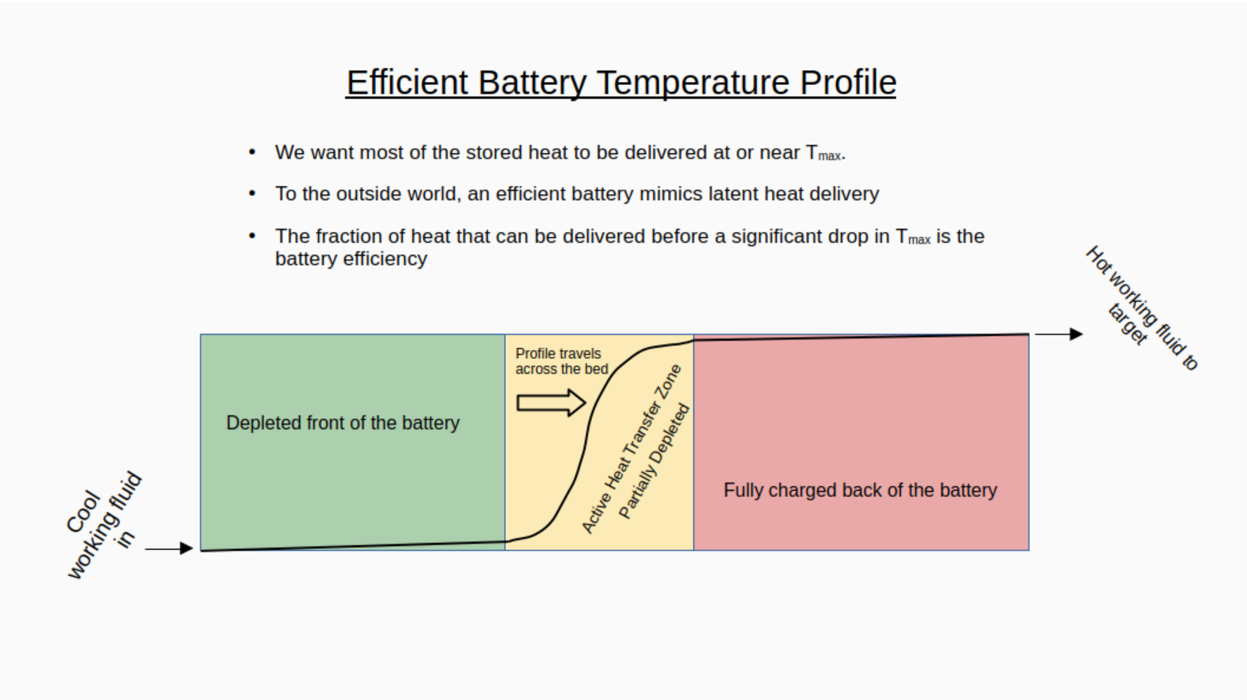

Table 1: *Cartoon of a high temperature thermal battery that is partly discharged and operates with a high efficiency temprature profile.*

There is much to do between here and a full featured model. I need to include bed pressure drop and do a proper estimate of model parameters as functions of temperature and pressure. We want a model that accounts for all the important physics, but neglects the unimportant physics. A model that accurately predicts battery performance and can guide our battery designs.

Nomenclature

All of they physical property and other parameters used in the model are in Table 1. I used a combination of Google, Grok, and Claude and, in the comments, I've tried to somewhat describe where (or how) I found (or calculated) the values. The dimensionless number values are at the bottom of the table.

Parameter	Description	Value	Units	Comment
Physical and Thermal Properties				
bed density	Overall Bed Density Including Solid and Gas	1440	kg/m3	
gas heat capacity		1200	J/kg K	estimated at 1200 K
K-eff	Effective Thermal Conductivity of the Bed	1.2	W/mK	Simple correction for porosity
k solid	Solid Thermal Conductivity	2	W/m K	Estimated for dense refractory at 1200 K
Porosity	Bed Porosity (void fraction)	0.4		Typical for packed bed
solid density		2400	kg/m3	Typical high Al, dense refractory
solid heat capacity		1270	J/kg K	estimated at 1200 K
T_max	Maximum Bed Temperature	2000	K	Maximum Bed Temperature
T_min	Minimum Bed Temperature	400	K	Minimum Bed Temperature
Radiation Properties				
Average Pressure	Average Bed Pressure (used for P*L calc)	2.00E+00	bara	
del	Distance Between Theoretical Radiative Plates	0.2	m	4*dp estimate for theoretical plate spacing
eps_eff for gas	Emmisivity of grey gas CO2	8.00E-02		Claude estimate confirmed by Grok
eps_s-g	Effective Emissivity for Gas Solid Radiative Heat Transfer	8.00E-02		Claude estimate by Grok -- gas resistance dominates
eps_solid	Emissivity of the Solid	0.8		Typical refractory emissivity
Mean path Length	Mean Path Length for solid-gas Radiative Interaction	3.99E-02	m	1.33 * dp * (1-porosity)
P*L	Path Length Time Pressure	7.98E-02	bar-m	The P*L for Hottel Charts
Sigma	Stefan Boltzman Constant	5.67E-08	W / m2 K4	Stefan Boltzman constant
Sigma *	Modified Stefan Boltzman for solid-solid Interaction	4.54E-08	W / m2 K4	Modified Stefan Boltzman Constant
SImga * g.s	Modified Stefan Boltzman for solid-gas Interaction	4.54E-09	W/m2 K4	
Geometric Properties				
C_a	Bed Cross Sectional Area	37.6	m2	
d_p	Particle Diameter	0.05	m	approximated to give a reasonable pressure drop
H	Height of the Bed	24.5	m	
L	Length of the Bed	6.13	M	
S_a	Bed Specific Surface Area	72	m2/m3	6*(1-eps)/dp
S_tot	Total Bed Surface Area	6.65E+04	m2	
V	Bed Volume	923	m3	
Flow and Transport Properties				
Bed delta-P	Pressure Drop Estimated at Gas Inlet Conditions	4.00E-03	Bar / m	estimate by Claude from Ergun equation
G, mass flux	Gas Mass Flux	1.04	kg/ m2 S2	per bed
h	Solid-Gas Convective Heat Transfer Coefficient	101	W / m2 K	Estimated by Claude using wakao Correlation
m_dot	Gas Mass Flow	39	Kg / S	Gas Mass Flow per bed
Dimensionless Groups				
C_p rat	Ratio of Gas to Solid Heat Capacity	9.45E-01		
N_cond	Inverse Bed Peclet Number for Conduction	1.49E-04		
N_conv	Ratio of Convective Capacity to Gas Carrying Capacity	1.43E+02		
N_g s rad	Ratio of Radiative Capacity to Gas Carrying Capacity	5.15E+01		
N_s s rad	Inverse Bed Peclet Number for Radiation	8.99E-03		

Table 1: *Physical and Thermal Properties, Radiation properties, Scoping Design Geometry Values*