$p(p, e^+\nu_e)d$ Astrophysical S factor by Monte Carlo Simulations of Photon Transport in Simple Stellar Models

C. Hsieh

Department of Physics, Hong Kong University of Science and Technology, Clear Water Bay, Hong Kong

A new approach using Monte Carlo Simulation is taken to determine the $p(p, e^+\nu_e)d$ astrophysical S factor from new developed simple stellar model and Clayton model. The results of new developed stellar model yields $7.5 \times 10^{-23} keV\ b$ and Clayton model yields $3.5 \times 10^{-15} keV\ b$, which is closed to the reference value of $(4.01 \pm 0.04) \times 10^{-22} keV\ b$. The small difference of the new developed stellar model with reference values shows that Monte Carlo photon simulation approach gives a good rough estimation of $S_{pp}(0)$ values and hence further confirms that $p.p.$ chain fusion dominates the nuclear reaction inside the sun.

After the missing neutrinos problems was resolved, a disagreement between observation and theoretical predictions of solar neutrino flux by Standard Solar Model (SSM), the solar neutrinos detection became a crucial methodology for the understanding of the sun. One important application of solar neutrinos is the calculation of nuclear S factor.[1] Nuclear S factor is one of the determining factors that affects the nuclear reaction rates inside the star. Currently, this factor is determined by fitting laboratory or observed data. However for $p.p.$ chain fusion reaction only high energy data are collected and used to estimate its S factor value.[2] The method of extrapolations to lower energies highly relies on the quality of high energy data.[2] This paper aims to develop a methodology to determine nuclear S factor theoretically inside the sun.

According to the SSM, $p.p.$ chain produces around 99% of the solar energy in the sun.[2] Therefore, the S factor determined theoretically would be the rate determining step inside the $p.p.$ chain which is represented as:

$$p + p \rightarrow d + e^{+} + \nu_e. \tag{1}$$

The S value would be denoted as S_{pp}. Astronomical S factor which has slow energy dependence, can be written in the form of Taylor Expansion and approximated by an energy independent constant $S_{pp}(0)$[2].

The main concept of this approach is to use the solar luminosity of the sun to deduce core energy production and hence calculate reaction rates. Then reaction rates is used to work backwards and find $S_{pp}(0)$. A simple stellar model would be created and obtained the density as a function of radius. The density is then used to calculate mean free path of photons and find out the delay factors for photons to diffuse out the radiative zone with respect to direct transfer. Surface luminosity is multiplied by this delay factor to find out core luminosity. The model developed referred as Model 1 would be compared with the Clayton's Stellar Model in prediction of $S_{pp}(0)$ values.

First, consider a homogenous sun consists of hydrogen. Since the radiation pressure of photons are far less than the pressure excreted by electron gas, radiation pressure can be ignored[3]. The electron density inside the sun is far less than the quantum concentration, so only classical pressure is needed to be considered[3]. By equating the ideal gas law and the pressure gradient due to self-gravity, the equation of the mass contained can be written as:

$$r^2 \frac{d^2M}{dr^2} - 2r\frac{dM}{dr} + wM\frac{dM}{dr} = 0 \tag{2}$$

where,

$$w = \frac{m_H}{kT}.$$

By rearranging the ideal gas law, the expression for temperature as a function of radius from core center (r) is:

$$T(r) = \frac{m_H}{k} \times \frac{1}{\rho(r,T)} \times \int -\rho(r,T)g\,dr \tag{3}$$

Equation (2) and (3) cannot be solved directly even by computers. Therefore, a self-consistent test was used to solve these coupled differential equations. First Equation (2) was solved by assuming the temperature is constant, and then $M_1(r)$ was found. By differentiating the mass and the density function $\rho_1(r)$ can then be obtained. Inputted the density into Equation (3), and found out the new temperature. This temperature was then used for the solving new round of solutions. However, even the constant temperature solution can't be solved directly, so a relationship of pressure gradient was introduced from the Clayton's model:

$$\frac{dP}{dr} = -\frac{4\pi}{3} G\rho_C^2 r e^{-\frac{r^2}{a^2}}. \tag{4}$$

2nd round of solutions were used to obtain the relationship of density as a function of radius (Appendix A1). The integration constants were fitted with boundary conditions. The boundary conditions are: at the solar radius the mass enclosed equals to solar mass, the core contains around 34% of solar mass[4], and density graph should be above 0 in the region. The results of the density graph are shown in Figure 1.

In order to find the core energy produced by nuclear fusion, a delay factor for photons to diffuse out the star is required. Inside the star, photons are mainly scattered by electron gases[3], and the density of electrons would further determines the mean free path of photons. The density of electrons can be found by the following relationships,

$$n_e = \frac{x\rho(r)}{m_H} \tag{5}$$

where x is fraction of electrons that is ionized and can be expressed as:

$$x \approx 10^{21} \times \frac{T^{\frac{3}{2}}}{n_e}\, e^{-\frac{158000}{T}} \tag{6}$$

For simplicity, by considering only the dominate process, Thompson scattering, the mean free path (l) of the photons can further be found as:

$$l = \frac{1}{n_e \sigma_T}, \tag{7}$$

where σ_T is the Thompson scattering cross section which equals to:

$$\sigma_T = \frac{8\pi}{3} \times \left(\frac{Ze^2}{4\pi\epsilon_0 m_e c^2}\right)^2 \quad . \tag{8}$$

The mean free path calculation was repeated for Clayton model's density profile (Figure 2) for comparison to Model 1.

Mean free path was used to input in a computer random walk simulation to find out the delay factor. Since the magnitude of mean free path is around 10^{-3} meters, and solar radius is in 10^{8} meter, it is impossible to do a direct simulation of random walk to determine the time for photons to escape from edge of center to the surface. A

Monte Carlo Simulation approach is then taken. It was observed that no matter how large the steps of the random walk were, the relationships between total number of steps and number of steps away from the certain point always follows the following relationship:

$$y = ax^b. \tag{9}$$

By determining how the parameters a and b change with respect to radius, one can construct the overall relationships between total steps and the steps away from the edge of core to the surface.

In the Monte Carlo simulation, the computer first random generated a distance R inside the solar radius, and this R was inputted inside the Mean Free Path function to determine the size of each random walk steps. Then the computer ran for $10^2, 10^3, 10^4, 10^5, 10^6$ steps and recorded its distance from the starting point. A log scale was taken on both axis and by determining the slope and intercept, one can obtain $b(r)$ and $blog(a)$ respectively. Also a plot between b and $log(a)$ was used to find out the relationships between the two parameters.

From Figure 3 and 4 it was observed that both b and $log(a)$ value is nearly constant throughout the solar radius. Therefore, it is not reliable to use these two figures to find out the radius dependence of these parameters. Surprisingly, Figure 5 shows a strong correlation between b and $log(a)$. A degree 4 polynomial was used to fit the data points. Since for any random walk the mean square distance (D) traveled in number of steps (N) can be expressed as:

$$D^2 = l_1^2 + l_2^2 + \cdots + l_N^2 \approx N l_{eff}. \tag{10}$$

Therefore,

$$D = a\sqrt{N} \tag{11}$$

where a is the square root of the effective mean free path (l_{eff}). Equation (11) predicts the b value to be 0.5, and by substituting b into the relationships in Figure 5, one can determine the a parameter.

Simply input number of steps from the edge of the core to surface (D) in Equation (11) and solve for the total number of steps required, then multiply by the time for each step, and the time for photon to diffuse out can then be determined. Divide the time for photons to travel through the solar radius, then the delay factor is obtained. Radiation diffusion would slow down the rate for energy to escape, thus the luminosity in the core would be larger than the surface luminosity by the delay factor. The core occupies around 0.2 solar radius[5]. Thus the power generated per unit volume inside the core can then be found. Assuming that the sun is generated by $p.p.$ chain fusion only, divide the average energy production by $p.p.$ chain, the $p(p, e^+\nu_e)d$ reaction rate can then be determined. Use the nuclear reaction rate equation (Equation 12), one can estimate the $p(p, e^{+}\nu_e)d$ Astrophysical S factor.

$$R_{AB} = 6.48 \times 10^{-24} \times \frac{n^2}{AZ^2} S(E_o) \left(\frac{E_G}{4kT}\right)^{\frac{2}{3}} e^{-3\left(\frac{E_G}{4kT}\right)^{\frac{1}{3}}} \quad (12)$$

The calculated $p(p, e^{+}\nu_e)d$ Astrophysical S factor for Model 1 and Clayton model are $7.5 \times 10^{-23} keV\ b$ and $3.5 \times 10^{-15} keV\ b$ respectively. The $p(p, e^{+}\nu_e)d$ reaction's $S(0)$ is around $(4.01 \pm 0.04) \times 10^{-22} keV\ b$[1]. Model 1 have results only 5 times less than the actual reference value, which shows that this approach gives a very good approximation in the nuclear S factor. As for the Clayton's model the S value prediction is more than 10^6 larger. The reason that Model 1 is better than Clayton's stellar model is that it considers the temperature effect in density and solved it by self consistent test. However, Clayton's model did not considers the coupled effect of temperature on density.

In this approach the highest uncertainty is the core region, it's in the range between $0.2 \sim 0.25$ solar core [1, 6]. Not only that the assumption of hydrogen homogenous sun, fusion by $p.p.$ chain only, photon scattering by Thompson scattering only and the input value of many parameters all contributed to the error. Even though the S value predictions by this approach is not as good as the experimental values, it provides an easy and pure theoretical approach to estimate the $S_{pp}(0)$ value inside the stars. Hence it further confirms that our sun is dominant by $p.p.$ chain fusion process.

Acknowledge: Special Thanks to Prof. P. Leung for supervising the project.

References:

[1]. F. Confortola, et al., Phys. Rev. C **75.**6 (2007)

[2]. E. G. Adelberger et al., Rev. Mod. Phys. **83**, 1 (2011)

[3]. A. C. Phillips, "Properties of Matter and Radiation." The Physics of Stars. 2nd ed. Chichester: Wiley, 1994. 65-66. Print.

[4]. Williams, R. David "Sun/Earth Comparison." Sun Fact Sheet. NASA, 13 Aug. 2015. Web

[5]. R. A. Garcia et al., Science 316.5831 (2007): 1591-593.

[6]. H. Hathaway, David. "The Solar Interior." NASA/Marshall Solar Physics. NASA, 1 Oct. 2015. Web

[7]. H. Hathaway,. David. "NASA/Marshall Solar Physics." NASA/Marshall Solar Physics. . David H. Hathaway,, 1 Oct. 2015. Web. 29 Nov. 2015.

Figures:

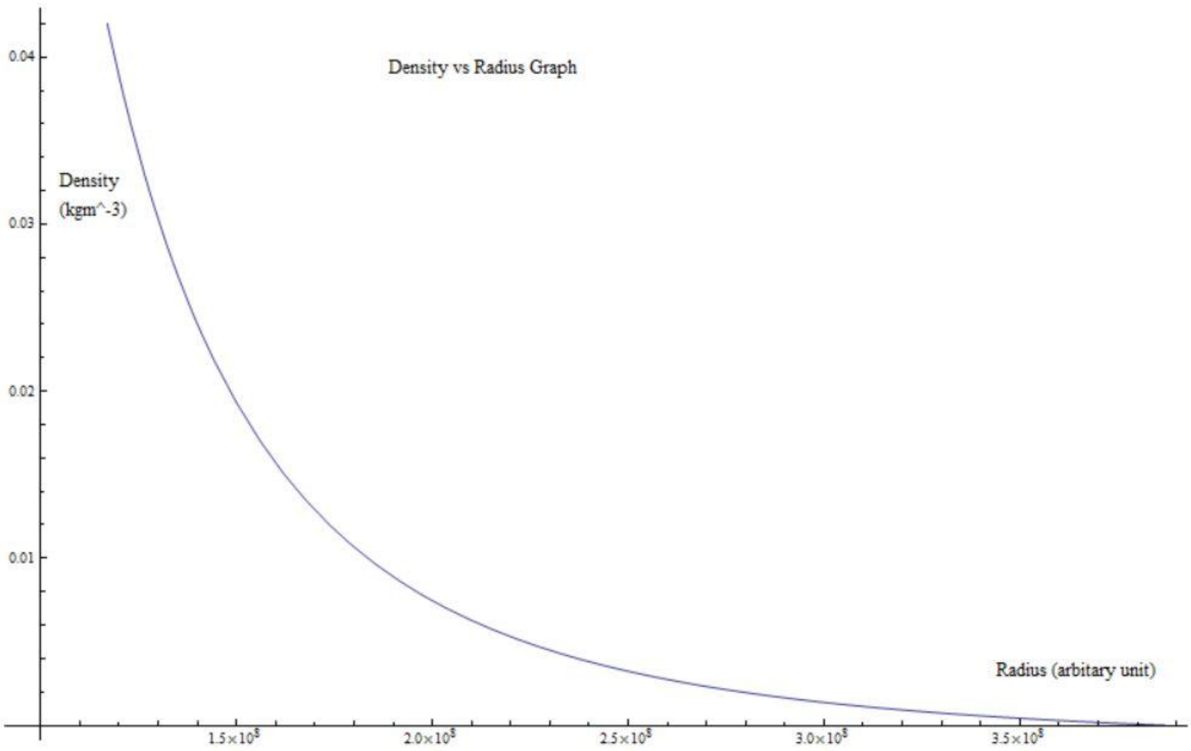
Density vs Radius Graph
Density
(kgm^-3)
0.04
0.03
0.02
0.01
Radius (arbitary unit)
1.5×10⁸
2.0×10⁸
2.5×10⁸
3.0×10⁸
3.5×10⁸

Fig 1.

C. Hsieh

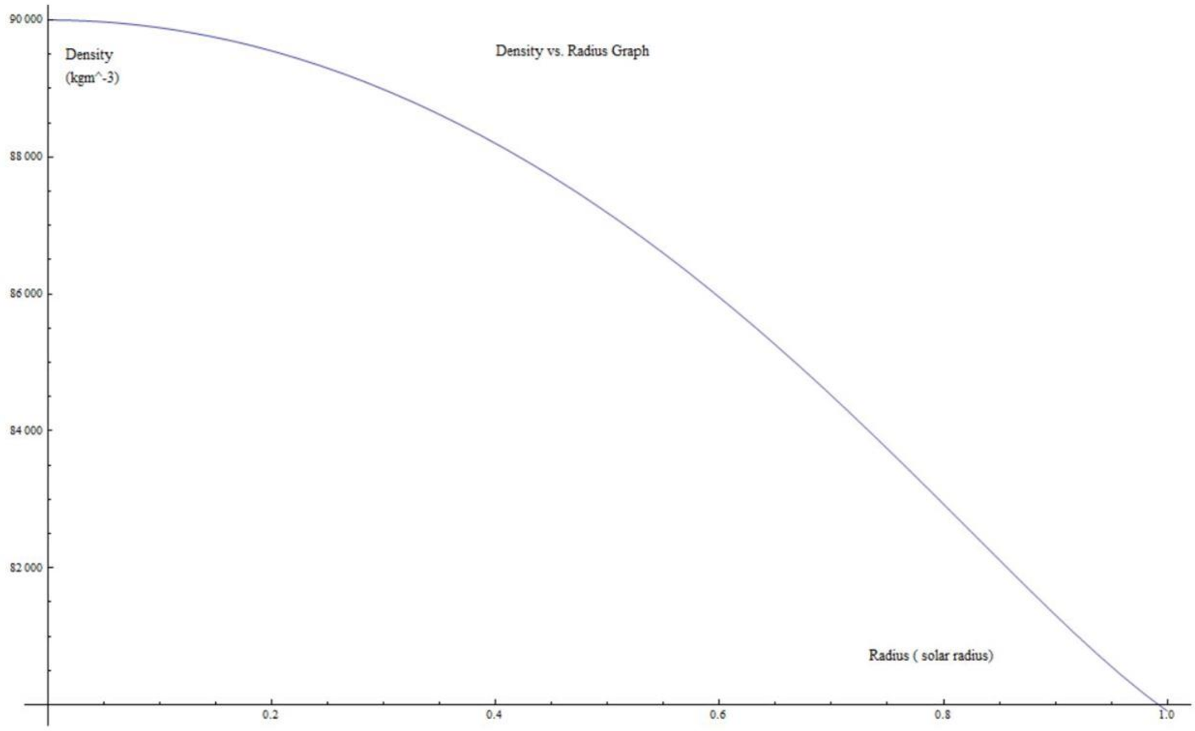
90 000
88 000
86 000
84 000
82 000
Density
(kgm^-3)
Density vs. Radius Graph
Radius (solar radius)
0.2
0.4
0.6
0.8
1.0

Fig 2.

C. Hsieh

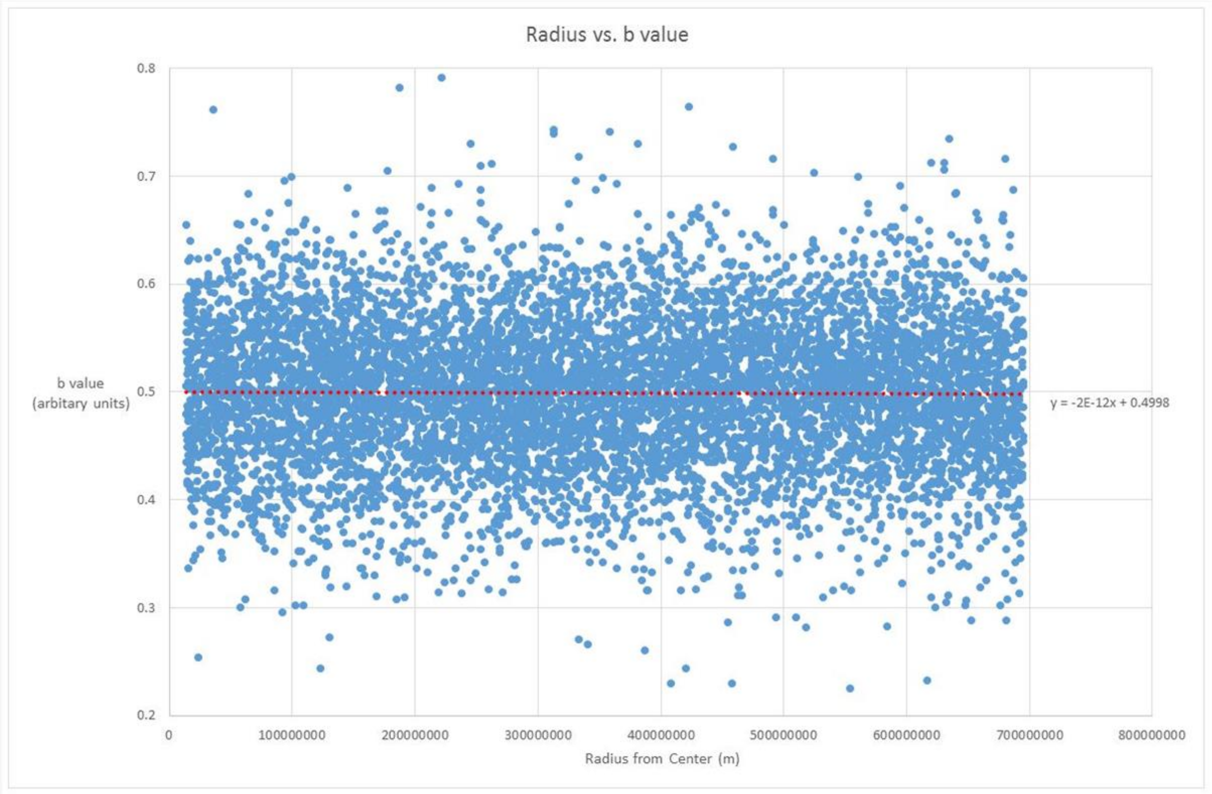
Radius vs. b value
b value
(arbitary units)
y = -2E-12x + 0.4998
Radius from Center (m)
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0
100000000
200000000
300000000
400000000
500000000
600000000
700000000
800000000

Fig 3.

C. Hsieh

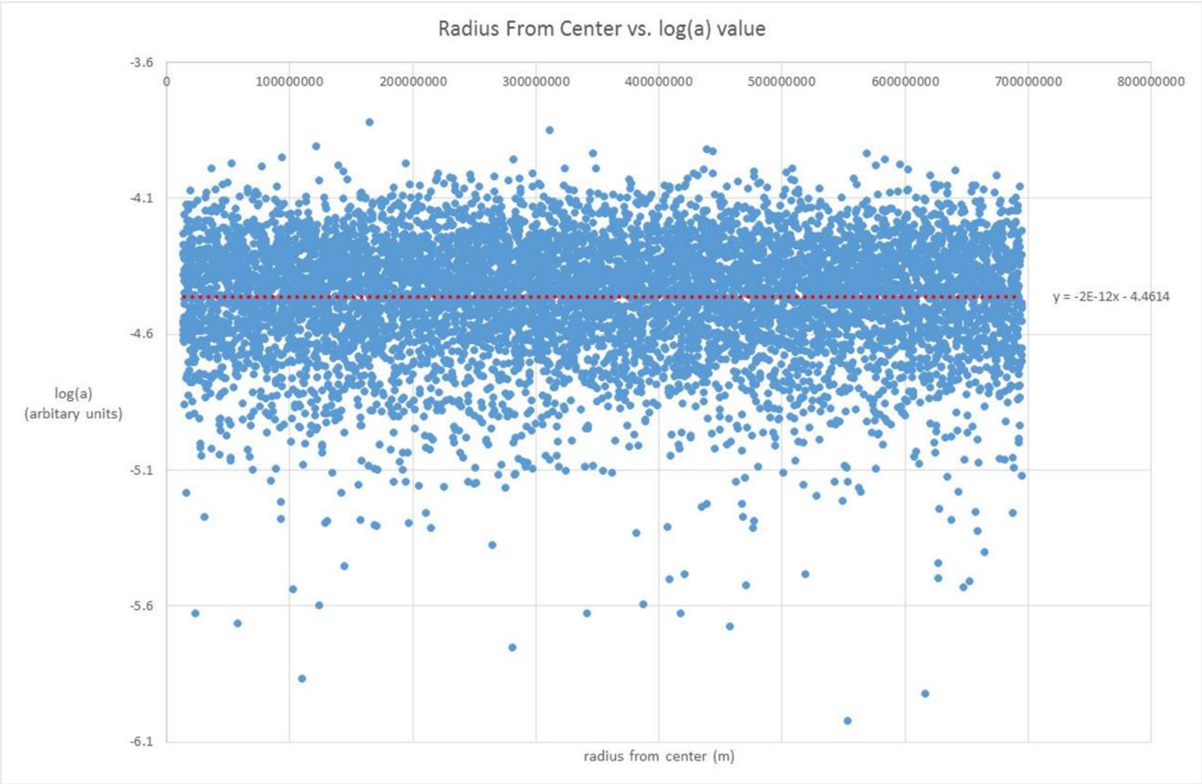
Radius From Center vs. log(a) value
-3.6
-4.1
-4.6
-5.1
-5.6
-6.1
0
100000000
200000000
300000000
400000000
500000000
600000000
700000000
800000000
y = -2E-12x - 4.4614
log(a)
(arbitary units)
radius from center (m)

Fig 4.

C. Hsieh

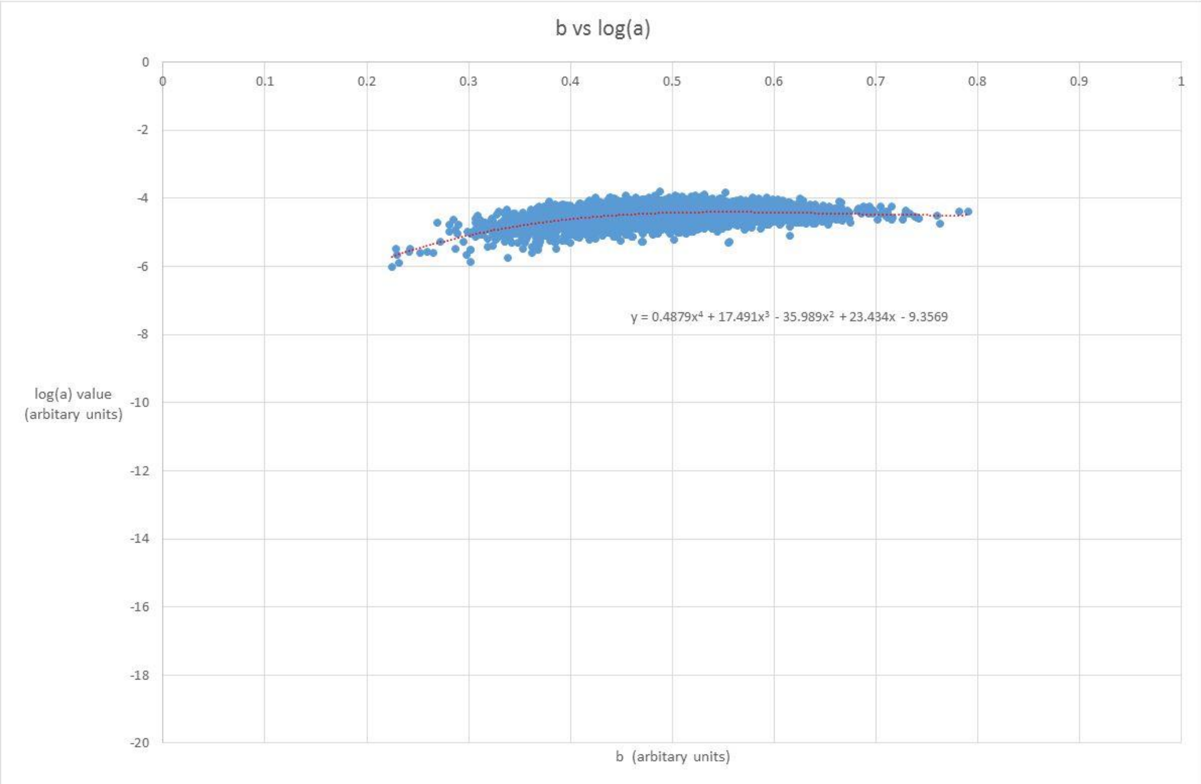
b vs log(a)
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
-2
-4
-6
-8
-10
-12
-14
-16
-18
-20
y = 0.4879x⁴ + 17.491x³ - 35.989x² + 23.434x - 9.3569
log(a) value
(arbitary units)
b (arbitary units)

Fig 5.

C. Hsieh

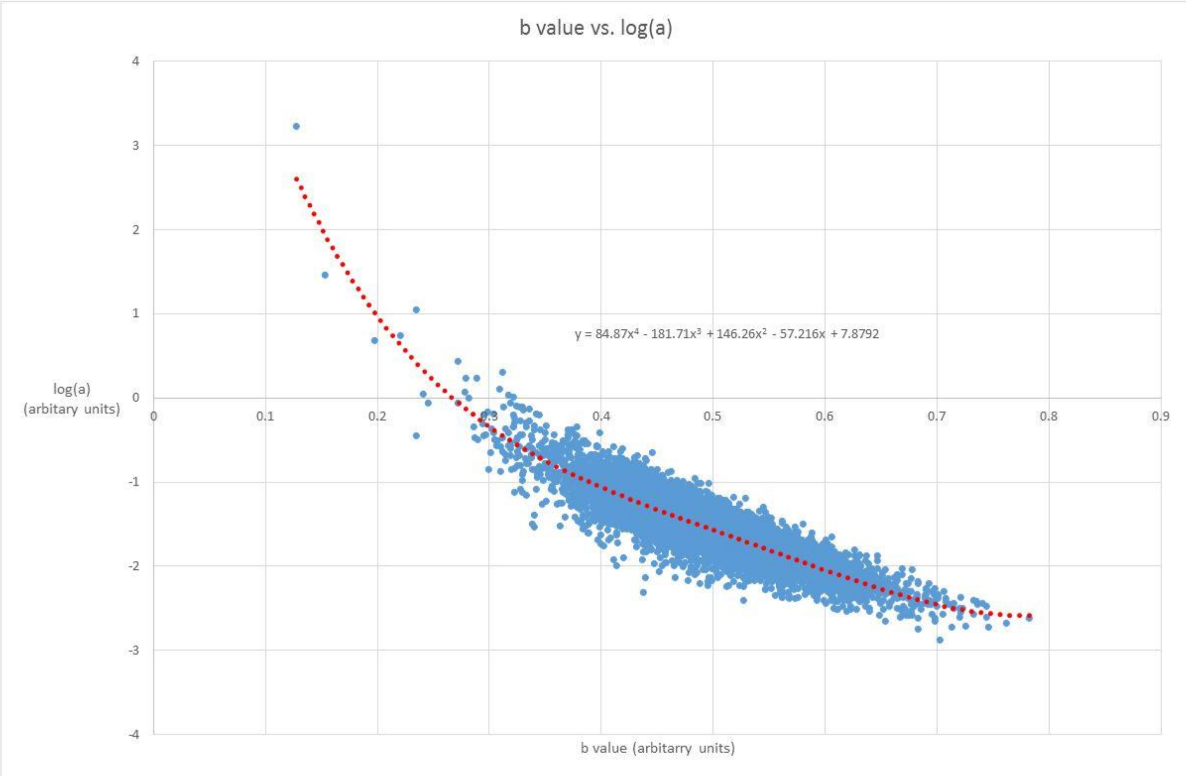
b value vs. log(a)
4
3
2
1
0
-1
-2
-3
-4
log(a)
(arbitary units)
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
y = 84.87x⁴ - 181.71x³ + 146.26x² - 57.216x + 7.8792
b value (arbitarry units)

Fig 6.

C. Hsieh

APPENDIX A

A1: Model 1. Density Analytical Solutions:

$$
\begin{aligned}
&\frac{1}{\pi r^2}\, 25\,000\,000\,000 \Bigg(-1.47458\times10^{-122}\, e^{6.01962\times10^{-17} r^2} \left(-\frac{1.65015\times10^{28}}{r^3} - 0.0000531507\, r \right) - 1.47458\times10^{-122}\, e^{6.01962\times10^{-17} r^2} \left(-\frac{1.28029\times10^{20}}{r^3} - 6.59802\times10^{-12}\, r \right) + \\
&\frac{8.71319\times10^{18}}{r} - \frac{1.32585\times10^{-117}\, e^{-6.01962\times10^{-17} r^2}}{r} + \frac{2.44124\times10^{-110}\, e^{6.01962\times10^{-17} r^2}}{r} - \frac{3 r^2}{100\,000\,000\,000} + 5.85669\times10^{-150}\, e^{-6.01962\times10^{-17} r^2} r^3 + 4.71788\times10^{-133}\, e^{6.01962\times10^{-17} r^2} r^3 - \\
&1.77529\times10^{-138}\, e^{6.01962\times10^{-17} r^2}\, r \left(-2.20739\times10^{11} + \frac{8.25075\times10^{27}}{r^2} - 0.0000265753\, r^2 \right) - 1.77529\times10^{-138}\, e^{6.01962\times10^{-17} r^2}\, r \left(27\,402.1 + \frac{6.40144\times10^{19}}{r^2} - 3.29901\times10^{-12}\, r^2 \right) + \\
&2.00694\times10^{-141}\, r^2\, \text{Erf}[7.75862\times10^{-9}\, r] + 1.6167\times10^{-124}\, r^2\, \text{Erfi}[7.75862\times10^{-9}\, r] - 5.68219\times10^{-118} \Bigg(\frac{1.\, \text{ExpIntegralEi}[-6.01962\times10^{-17} r^2]}{r} + \frac{2.\, e^{-6.01962\times10^{-17} r^2}\, \text{Log}[7.75862\times10^{-9}\, r]}{r} - \\
&2 \Bigg(\frac{1.}{r} - 6.01962\times10^{-17} r^2 \Bigg(-\frac{0.5\, (\text{HypergeometricPFQ}[\{1, 1\}, \{2, 2\}, -6.01962\times10^{-17} r^2] - \text{HypergeometricPFQ}[\{1, 1, 1\}, \{2, 2, 2\}, -6.01962\times10^{-17} r^2])}{r} + \\
&\frac{8.30617\times10^{15} \left(\frac{2.}{r} - \frac{2.\, e^{-6.01962\times10^{-17} r^2}}{r} \right) \text{Log}[7.75862\times10^{-9}\, r]}{r^2} + \frac{8.30617\times10^{15}\, (\text{EulerGamma} + \text{Gamma}[0, 6.01962\times10^{-17} r^2] + \text{Log}[6.01962\times10^{-17} r^2])}{r^3} - \\
&\frac{1.66123\times10^{16}\, \text{Log}[7.75862\times10^{-9}\, r]\, (\text{EulerGamma} + \text{Gamma}[0, 6.01962\times10^{-17} r^2] + \text{Log}[6.01962\times10^{-17} r^2])}{r^3} \Bigg) - 1.20392\times10^{-16}\, r \Bigg(-\frac{1}{4}\, \text{HypergeometricPFQ}[\\
&\{1, 1, 1\}, \{2, 2, 2\}, -6.01962\times10^{-17} r^2] + \frac{8.30617\times10^{15}\, \text{Log}[7.75862\times10^{-9}\, r]\, (\text{EulerGamma} + \text{Gamma}[0, 6.01962\times10^{-17} r^2] + \text{Log}[6.01962\times10^{-17} r^2])}{r^2} \Bigg)\Bigg)\Bigg)\Bigg)
\end{aligned}
$$

A2. Clayton Model Density Function:

$$D(r) = 90000x^3 \sqrt{\frac{e^{-x^2}}{x^6 - \frac{3x^5}{4} + \frac{3x^{10}}{10} - \frac{x^{12}}{12}}}$$

Where $x = \frac{r}{R_{sun}} \times 5.4$

APPENDIX B

B1: Input factors used for modeling:

Table I: *Input Factors used for Model 1*

Quantity	Value
Mass of Sun ($10^{24}\ kg$)	1,988,500[¶]
Radius of Sun (km)	696000[¶]
Core Size upper limit ($solar\ radius$)	0.25[†]
Core Size lower limit ($solar\ radius$)	0.2[*]
Radiative Zone Mean Temperature (K)	$4.5\ \times 10^{6}$[*]
Energy Produced by $p.p.$ chain (MeV)	15[‡]
Solar Surface Luminosity ($10^{26}\ W$)	3.846[¶]
Gamow Energy for $p.p.$ chain (eV)	493[‡]
Core Temperature (K)	$1.55\ \times 10^{7}$[¶¶]

[¶¶] E. G. Adelberger et al., Rev. Mod. Phys. **83**, 1 (2011)

[¶] Williams, R. David "Sun/Earth Comparison." Sun Fact Sheet. NASA,

[†] H. Hathaway,. David. "NASA/Marshall Solar Physics."

[‡] A. C. Phillips, The Physics of Stars. 2nd ed.

[*] R. A. Garcia et al., Science 316.5831 (2007)

B2: Model Predictions Comparison:

Table II: *Comparison between Model 1, Clayton Model and Reference Value*

Quantity	Model 1	Clayton model	Reference Value
Core Density (kgm^{-3})	8.5×10^6	9×10^4	1.5×10^5 †
Time Diffuse Out (s)	430.17	2.12×10^8	NA¶
Nuclear Power per unit Volume (Wm^{-3})	6307.5	3.119×10^9	120 ‡
Reaction Rate $(m^{-3}s^{-3})$	1.47×10^{15}	7.29×10^{20}	5×10^{13} ‡
Nuclear S factor $(keV\ barns)$	7.5×10^{-23}	3.5×10^{-15}	4.01×10^{-22} *

¶ Williams, R. David "Sun/Earth Comparison." Sun Fact Sheet. NASA,

† H. Hathaway,. David. "NASA/Marshall Solar Physics."

‡ A. C. Phillips, The Physics of Stars. 2nd ed.

* F. Confortola, et al., Phys. Rev. C **75**.6 (2007)