Pade order investigation

Asym vs. FESEM thickness or Rate

-0.5σ to $+2\ \sigma$, bkg subtract

Run 1 data

x-error bars turned into y-errors

Pade approximates

In mathematics a **Padé approximant** is the "best" approximation of a function by a rational function of given order.

Given a function *f* and two integers *m* ≥ 0 and *n* ≥ 1, the *Padé approximant* of order [m/n] is the rational function

$$R(x) = \frac{\sum_{j=0}^{m} a_j x^j}{1 + \sum_{k=1}^{n} b_k x^k} = \frac{a_0 + a_1 x + a_2 x^2 + \cdots + a_m x^m}{1 + b_1 x + b_2 x^2 + \cdots + b_n x^n}$$

Taylor series expansions are one example of Pade’ (Pade (1,0), Pade (2,0), Pade(3,0)…

The typical fitting function $A = \frac{Ao}{1+\gamma T}$ is also Pade’ (0,1)

F testing

- The goodness of a fit is typically found by looking at reduced χ^2 or reduced R^2, which show how far the fit is from the data
- It is possible to overfit functions looking only at these "goodness of fit" tests
- An "F-test" can be used to see, to a given degree of confidence, if adding the next order term in an expansion is justified. If the F-test fails, there is a n% chance that the term isn't needed

$$F = \frac{S_{j-1} - S_j}{S_j}(N - j - 1)$$

is distributed as a Fisher–Snedecor $F(1, N - j - 1)$ variable if the j^{th} degree is not justified.

From the tabulated value of the F distribution one can then give the prescription in Table 10.2.

Table 10.2. Maximum degree needed in polynomial approximation.

$N - j - 1$	2	3	4	6	8	12	20	60	120
Reject j^{th} order to 95% confidence level if F is smaller than	18.5	10.1	7.7	6	5.3	4.7	4.3	4	3.9

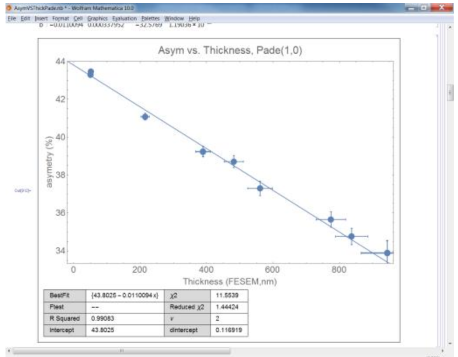
Comparison of fitting functions for asymmetry zero thickness extrapolation

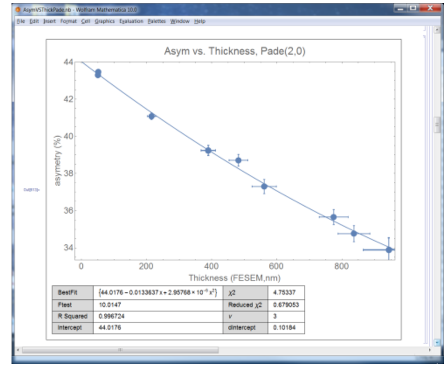
- Two ways to look at data
  - Asymmetry vs. Thickness
    - Asymmetry using Daniel's best data: -0.5σ - +2.0 σ, background subtracted
    - FESEM thickness, 500 nm point fixed to best average
  - Asymmetry vs. Rate

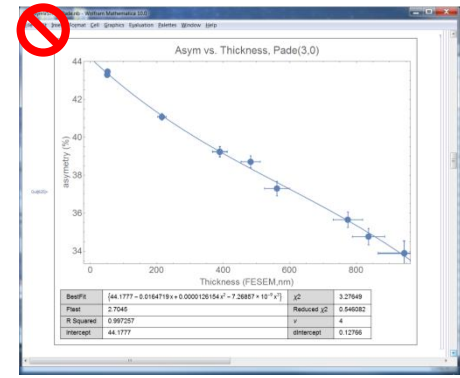
Typical fitting functions

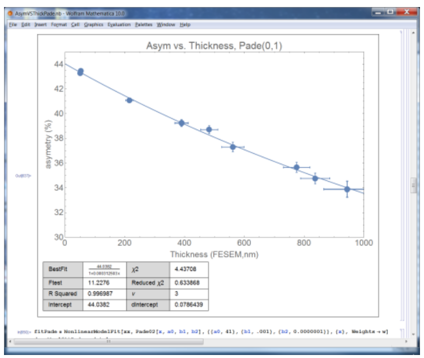
- $A = \frac{Ao}{1+\gamma T}$ is nonlinear, but can be linearized by inverting to $\frac{1}{A}$ =a+bT, where T is thickness and A is asymmetry
- Thickness vs. rate ~ quadratic (needs second order for thicker foils to fit reasonably well)
  - $R = c \cdot T + d \cdot T^2$, leading to T= $c' + d' \cdot R^{1/2}$ or $\frac{1}{A}$ =a+bR^n
- Plot two different things to varying Pade orders
  - A vs. T
  - 1/A vs. Rate

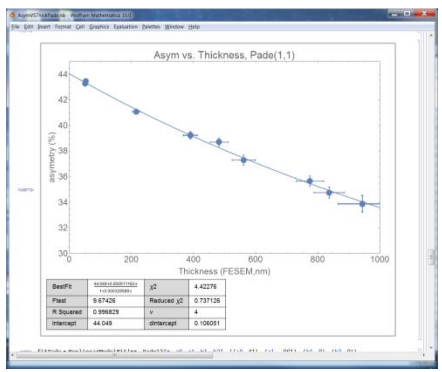
Asymmetry vs. Thickness

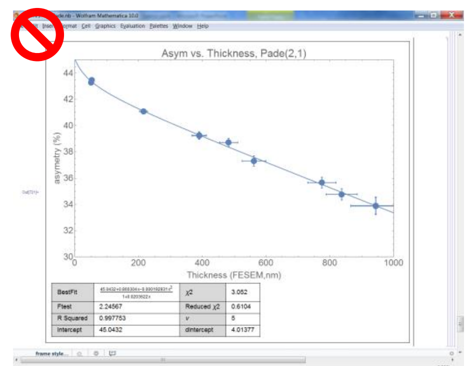


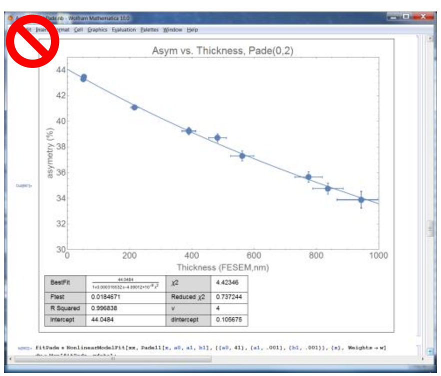


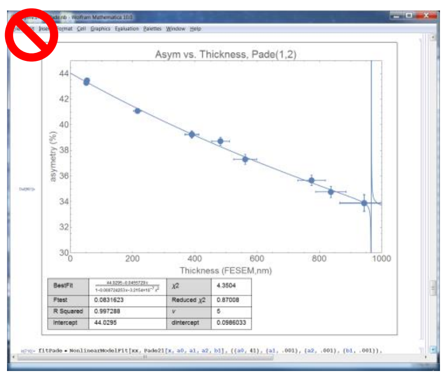










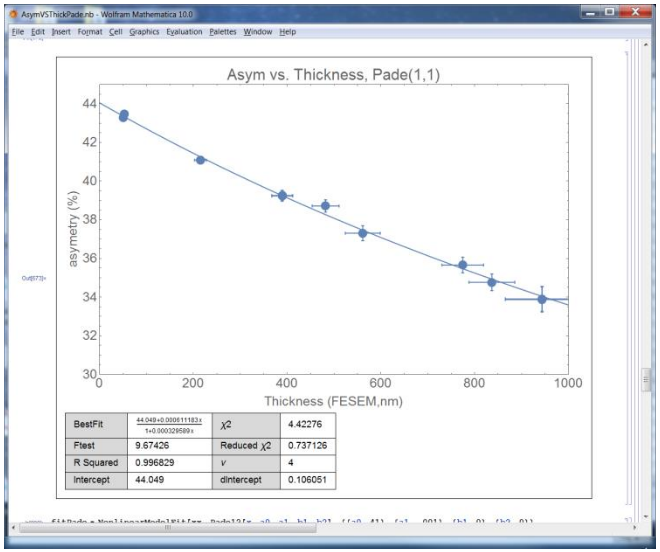


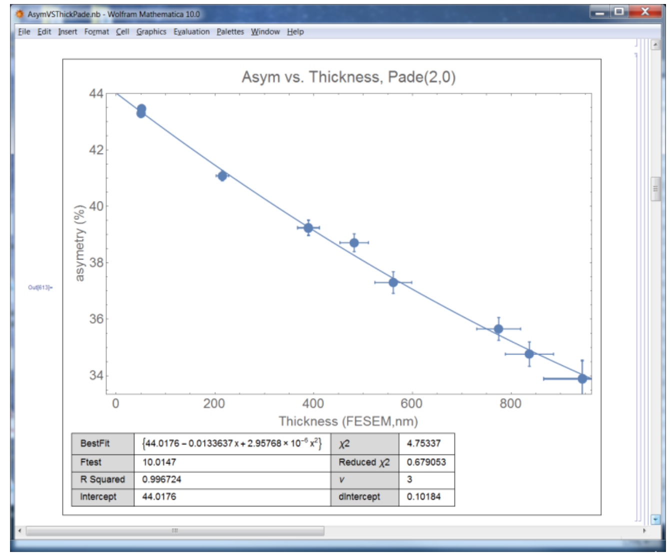
Y error bars have been manipulated to have the x uncertainty included since mathematical typically only fits with y uncertainty. Pade (0,1) (typical fit) used to transform error bars

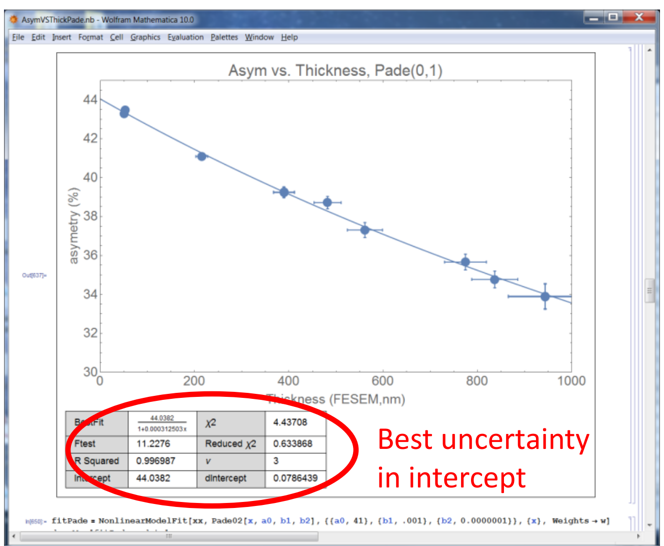
Pade(n,m) orders: Asy vs. Thick

Pade(n,m)	intercept	dA	R^2	red. χ^2	Ftest
(1,0)	43.8025	0.1169	0.991	1.44	-- worst red. χ^2
(2,0)	44.0176	0.1018	0.997	0.679	10.01
(3,0)	~~44.1777~~	0.128	0.997	0.546	2.70 (rej F test)
(0,1)	44.0382	0.0786	0.997	0.634	11.23
(0,2)	~~44.0484~~	0.1057	0.997	0.737	0.0185 (rej ftest)
(1,1)	44.049	0.1061	0.997	0.737	9.67
(1,2)	~~44.0295~~	0.0986	0.997	0.870	0.083 (rej. Ftest)
(2,1)	~~44.043~~	4.014	0.998	0.6104	2.24 (rej. Ftest)

Potential fits: not statistically rejected







Pade(n,m)	Asym(%)	dA	
(2,0)	44.0176	0.1018	
(0,1)	**44.0382**	**0.0786**	**Normal fit**
(1,1)	44.049	0.1061	
averaged	**44.0352**	**0.0537**	***Additional uncertainty due to model***

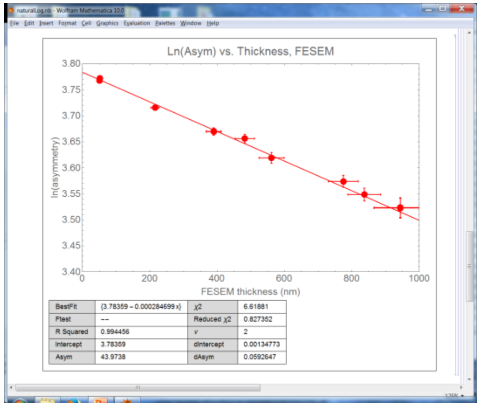
Zero thickness extrapolation largely independent of fit function used, assuming statistically reasonable fits

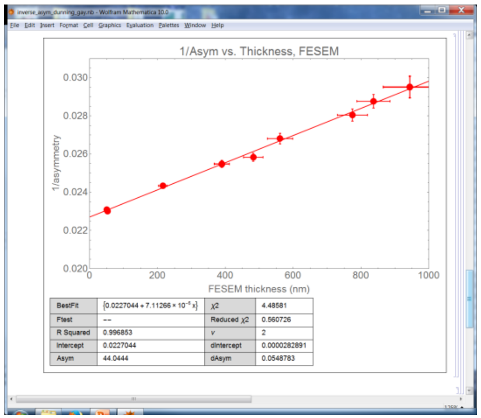
Other functional forms for fit?

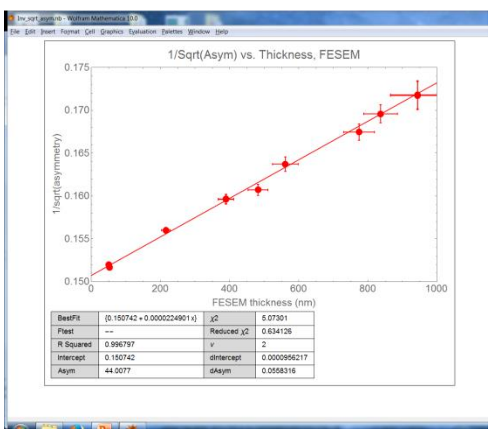
Other functional forms have been used historically to fit asym. vs. thickness

- $\ln(A)\ vs\ T$
- $\frac{1}{A}\ vs\ T$ (similar to inverting standard)
- $\frac{1}{\sqrt{A}}\ vs\ T$

Pade(n,m)	Asym(%)	dA	
ln(A)	43.914	0.059	
1/A	44.044	0.0549	Normal fit
1/√A	44.008	0.0558	



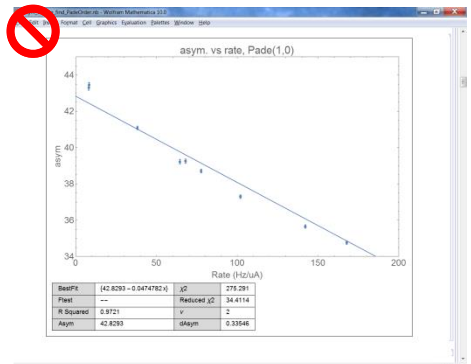


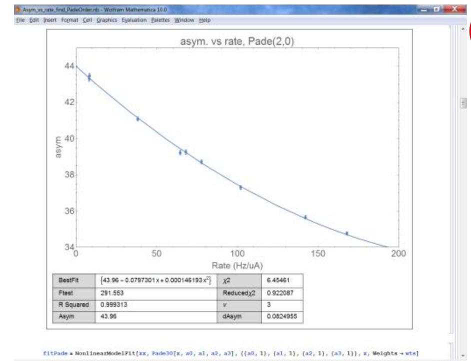


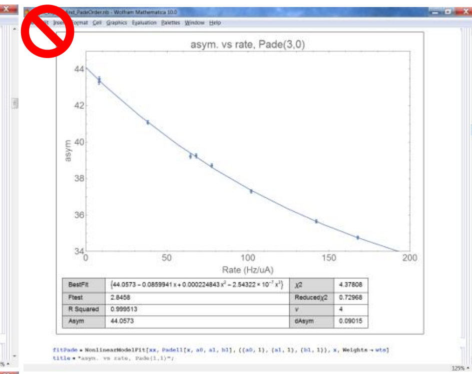
Consider Asym vs. Rate instead?

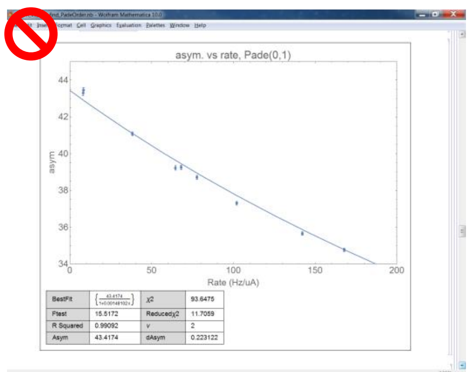
- Plot Asymmetry vs. average detector rate
- Run one data only thus far, “gold” cuts
  - -0.5σ to +2 σ, bkg subtract
  - x-error bars turned into y-errors (using Pade (1,1))
- Fitted Pade(n,m) orders until F test started failing

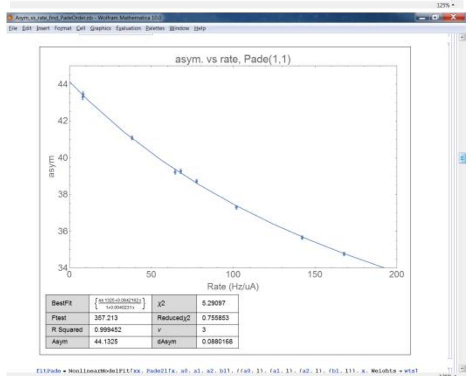
Pade orders: Asym vs. Rate

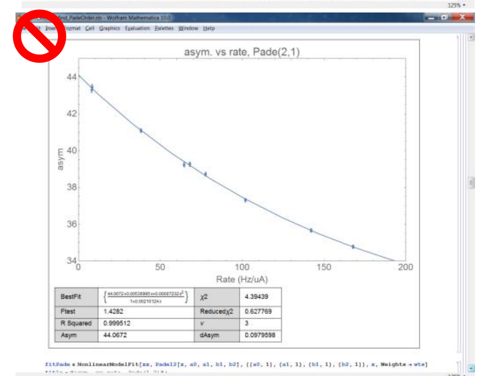


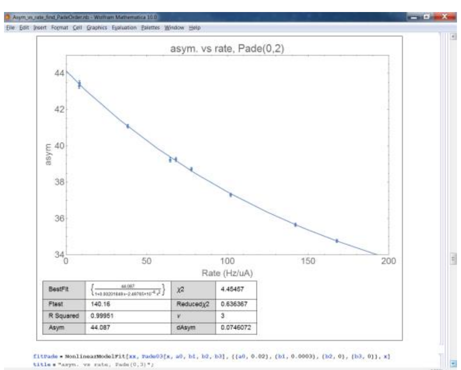


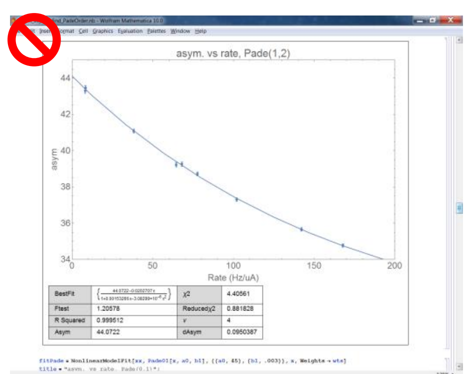


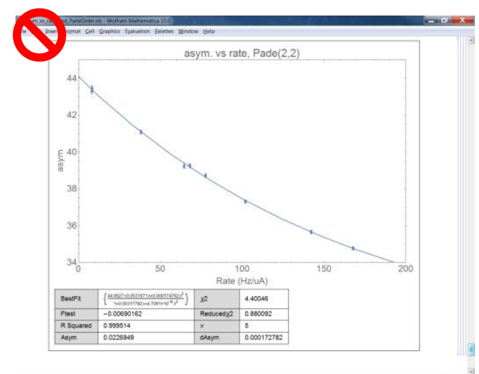












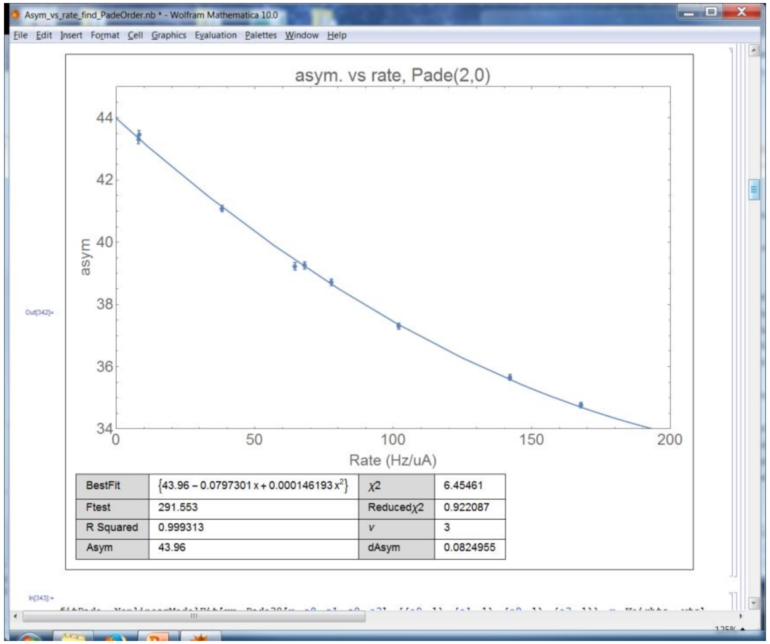
Again, rate uncertainty extrapolated to asym uncertainty for fitting. Rate uncertainties much smaller percentage than thickness uncertainties

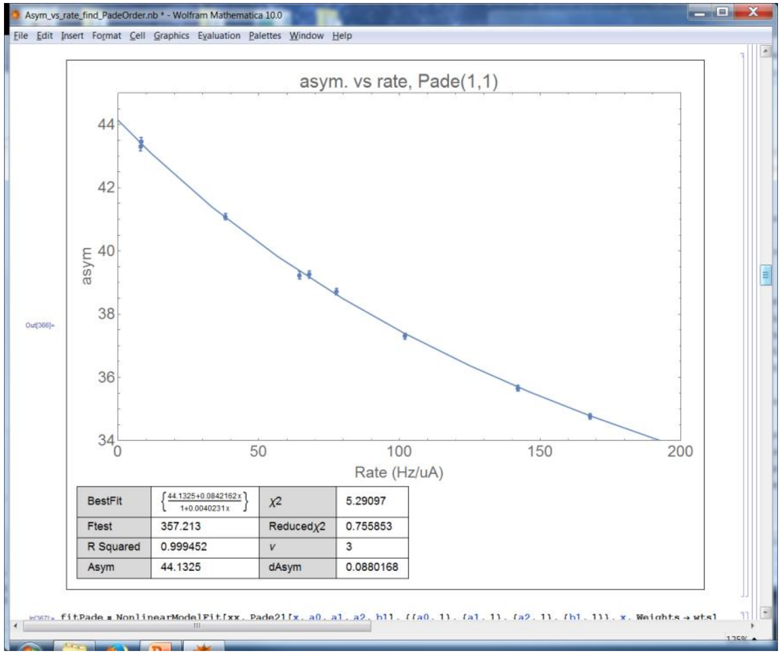
Pade(n,m) orders: 1/A vs rate

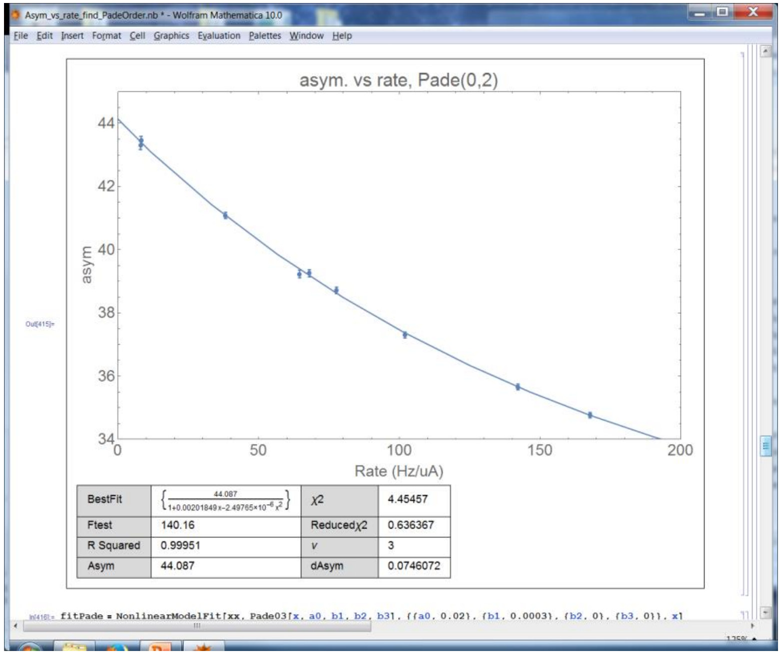
Pade(n,m)	intercept	dA	R^2	red. χ^2	Ftest	
(1,0)	~~42.8~~	.33	.97	35	--	Reject chi
(2,0)	43.96	.082	.999	0.922	291	
(3,0)	~~44.06~~	.090	.999	0.930	2.84	Reject F
(1,1)	44.133	.088	.999	0.756	357	
(2,1)	~~44.067~~	.098	.999	0.628	1.42	Reject F
(1,2)	~~44.072~~	.095	.999	0.882	1.20	Reject F
(0,1)	~~43.42~~	.0223	.991	11.7	15.51	Reject chi
(0,2)	44.087	0.075	.999	0.636	140.2	
(0,3)	--				Not converge	
(2,2)	~~44.057~~	.156	.999	0.73	0.013	Reject F

Viable fits: A vs. R

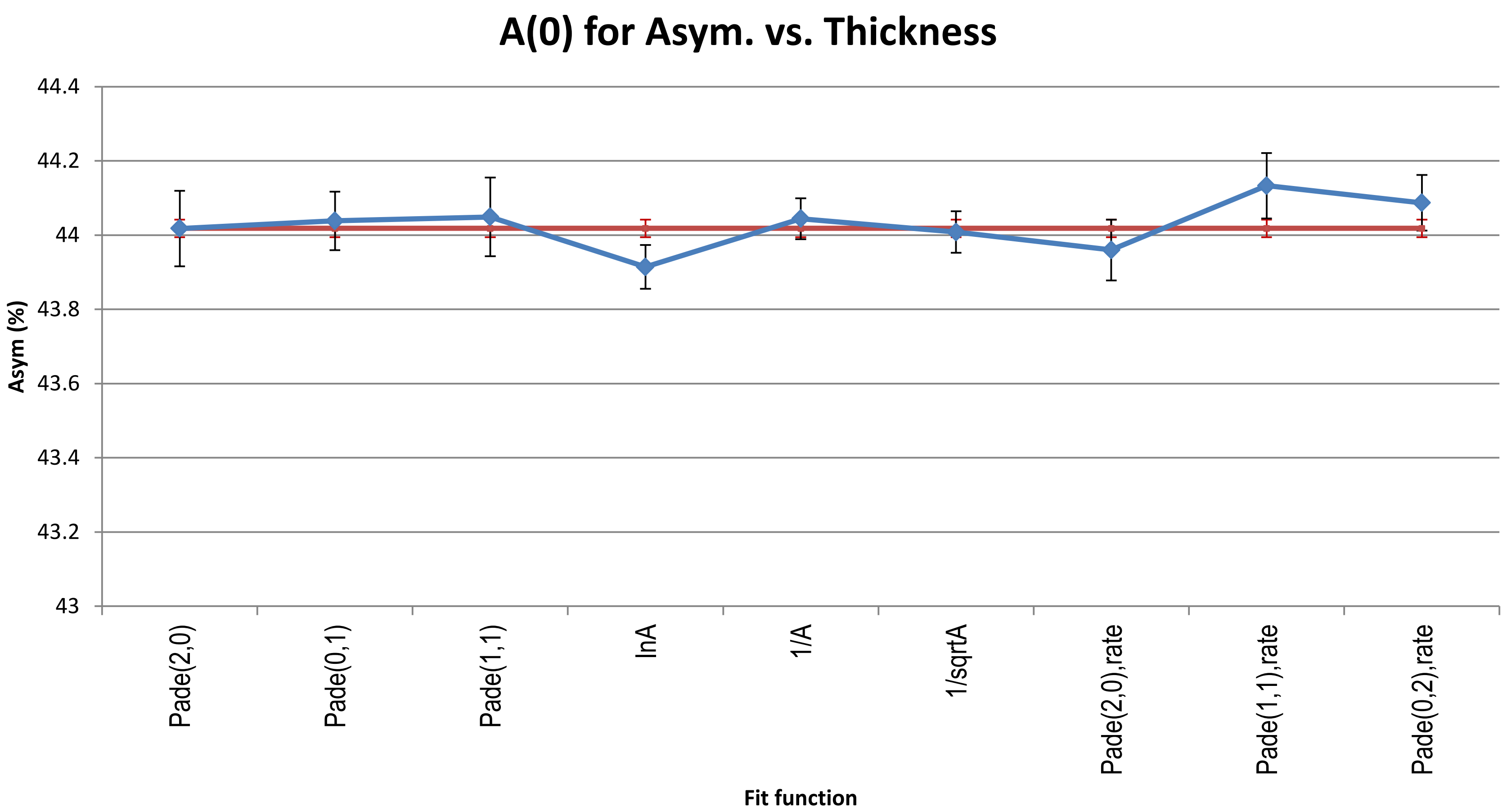
Pade(n,m)	intercept	dA
(2,0)	43.96	.082
(1,1)	44.133	.088
(0,2)	44.087	0.075
average	44.058	0.047







All potential good fits(blue) and average with uncertainty (red)



Conclusions

- Fitting A vs. T: std. fit form gives lowest uncertainties
- Use Pade analysis, F-testing to determine other viable functional forms
- Fitting A vs. Rate: 3 forms have viable fits, uncertainties all comparable to best in A vs. T
- Translating x uncertainties to y axis (done by root, this mathematica analysis) requires model dependence, likely not a large error factor.