MODELS FOR FITTING REFRACTIVE INDEX n vs. λ

Preferred equations are highlighted in GREEN. They have been identified as the most common equations used for interpolation in several optical design programs or in books dealing with optical properties of materials.

There are many equations that have been used to represent the index of refraction of optical materials as a function of wavelength. The earliest is the Cauchy equation, which dates back to 1836. Both Jenkins & White and Ditchburn show the following general form:

$$n(\lambda) = A + \frac{B}{\lambda^2} + \frac{C}{\lambda^4} + \cdots$$

EQN NAME	EQUATION	NOTES
CAUCHY	$n(\lambda) = A + \frac{B}{\lambda^2} + \frac{C}{\lambda^4}$	Refs: Smith, Angewandte used by TFCalc

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Another group contains the **CONRADY** equations. These simple models are often used to fit sparse data. The first appeared in Conrady's book "Applied Optics and Optical Design (p. 659).

EQN NAME	EQUATION	NOTES
CONRADY1	$n(\lambda) = \mathrm{A} + \frac{\mathrm{B}}{\lambda} + \frac{\mathrm{C}}{\lambda^{3.5}}$	Refs: Smith, Angewandte used by OSLO, Opticad, TracePro, ZEMAX
CONRADY2	$n(\lambda) = \mathrm{A} + \frac{\mathrm{B}}{\lambda^2} + \frac{\mathrm{C}}{\lambda^{3.5}}$	

There is a family of equations based upon work by **HELMHOLTZ**. Jenkins & White show:

$$n(\lambda)^2 = A_o + \sum_{i=1}^{m} \frac{A_i \lambda^2}{(\lambda^2 - \lambda_i^2) + B_i \lambda^2 / (\lambda^2 - \lambda_i^2)}$$

These equations are based on physical principles and can be very complex. They are rarely seen today.

The **HARTMANN** equation has the general form:

$$n(\lambda) = A + \frac{B}{(C-\lambda)^D}$$

where the exponent D assumes values between 1 and 2.

EQN NAME	EQUATION	NOTES
HARTMANN 1	$n(\lambda) = A + \frac{B}{(C-\lambda)}$	used by TFCalc
HARTMANN 2	$n(\lambda) = A + \frac{B}{(C-\lambda)^2}$	used by TFCalc

Hartmann equations also appear in the following refs:

EQN NAME	EQUATION	NOTES
HARTMANN3a	$n(\lambda) = A + \frac{B}{(C-\lambda)^{1.2}}$	Ditchburn
HARTMANN3b	$n = \frac{A}{(\lambda - B)^{1.2}}$	Luneberg
HARTMANN4	$n(\lambda) = A + \frac{B}{(C-\lambda)} + \frac{D}{(E-\lambda)}$	Smith and Angewandte

HERZBERGER devised a useful equation for fitting over wide wavelength ranges. It comes in many guises. The first is a 4-term Herzberger equation. The constant 0.028 represents a short wavelength corresponding to the high frequency absorption edge, which is valid for a wide class of materials.

From this point we may add or subtract terms as needed. Five-term and six-term Herzberger equations are quite common. It is also possible to change the constant 0.028 into variables K and L, and the number 0.035 is occasionally seen.

EQN NAME	EQUATION	NOTES
HERZBRGR2X2	$n(\lambda)=A+B\lambda^2+\frac{C}{(\lambda^2-0.028)}+\frac{D}{(\lambda^2-0.028)^2}$	Smith and Angewandt use 0.035 here
HERZBRGR3X2	$n(\lambda)=A+B\lambda^2+C\lambda^4+\frac{D}{(\lambda^2-0.028)}+\frac{E}{(\lambda^2-0.028)^2}$	Laikin; used for LiF and Irtran2
HERZBRGR4X2	$n(\lambda)=A+B\lambda^2+C\lambda^4+D\lambda^6+\frac{E}{(\lambda^2-0.028)}+\frac{F}{(\lambda^2-0.028)^2}$	used by ZEMAX, Optalix, TracePro, Opticad
HERZBRGR3X3	$n(\lambda)=A+B\lambda^2+C\lambda^4+\frac{D}{(\lambda^2-0.028)}+\frac{E}{(\lambda^2-0.028)^2}+\frac{F}{(\lambda^2-0.028)^2}$	
HERZBRGR5X2	$n(\lambda)=A+B\lambda^2+C\lambda^4+D\lambda^6+E\lambda^8+\frac{F}{(\lambda^2-0.028)}+\frac{G}{(\lambda^2-0.028)^2}$	
HERZBGRJK	$n(\lambda)=A+B\lambda^2+C\lambda^4+D\lambda^6+\frac{E}{(\lambda^2-J)}+\frac{F}{(\lambda^2-K)^2}$	J and/or K could be 0.035 or a variable

SCHOTT Glasswerke devised a useful polynomial equation based on a Laurent series that has several variants. The simplest has 5-terms. Better results are often achieved by adding more terms. A 6-term Schott equation, is most common. A 7-term Schott equation is occasionally seen. Schott Glass abandoned these formulae in 1992, and switched to a Sellmeier representation. These are still in widespread use elsewhere.

EQN NAME	EQUATION	NOTES
SCHOTT2X3	$n(\lambda)^2 = \mathrm{A} + \mathrm{B}\lambda^2 + \frac{C}{\lambda^2} + \frac{\mathrm{D}}{\lambda^4} + \frac{\mathrm{E}}{\lambda^6}$	
SCHOTT2X4	$n(\lambda)^2 = \mathrm{A} + \mathrm{B}\lambda^2 + \frac{C}{\lambda^2} + \frac{\mathrm{D}}{\lambda^4} + \frac{\mathrm{E}}{\lambda^6} + \frac{F}{\lambda^8}$	Ref Smith as "Old Schott" used by ZEMAX, OSLO, Optalix, TFCalc, TracePro, Opticad. Laikin 0
SCHOTT2X5	$n(\lambda)^2 = \mathrm{A} + \mathrm{B}\lambda^2 + \frac{C}{\lambda^2} + \frac{\mathrm{D}}{\lambda^4} + \frac{\mathrm{E}}{\lambda^6} + \frac{F}{\lambda^8} + \frac{G}{\lambda^{10}}$	Ref Angewandte, called glasherstellar
SCHOTT2X6	$\mathrm{n}(\lambda)^2 = \mathrm{A} + \mathrm{B}\lambda^2 + \frac{C}{\lambda^2} + \frac{\mathrm{D}}{\lambda^4} + \frac{\mathrm{E}}{\lambda^6} + \frac{F}{\lambda^8} + \frac{G}{\lambda^{10}} + \frac{H}{\lambda^{12}}$	Extended in Zemax
SCHOTT3X3	$\mathrm{n}(\lambda)^2 = \mathrm{A} + \mathrm{B}\lambda^2 + \mathrm{C}\lambda^4 + \frac{D}{\lambda^2} + \frac{\mathrm{E}}{\lambda^4} + \frac{\mathrm{F}}{\lambda^6}$	Laikin 3 = polynomial
SCHOTT3X4	$\mathrm{n}(\lambda)^2 = \mathrm{A} + \mathrm{B}\lambda^2 + \mathrm{C}\lambda^4 + \frac{D}{\lambda^2} + \frac{\mathrm{E}}{\lambda^4} + \frac{\mathrm{F}}{\lambda^6} + \frac{G}{\lambda^8}$	Ref Angewandte, called glasherstellar
SCHOTT3X5	$\mathrm{n}(\lambda)^2 = \mathrm{A} + \mathrm{B}\lambda^2 + \mathrm{C}\lambda^4 + \frac{D}{\lambda^2} + \frac{\mathrm{E}}{\lambda^4} + \frac{\mathrm{F}}{\lambda^6} + \frac{G}{\lambda^8} + \frac{H}{\lambda^{10}}$	Ref Angewandte, called glasherstellar
SCHOTT4X4	$\mathrm{n}(\lambda)^2 = \mathrm{A} + \mathrm{B}\lambda^2 + C\lambda^4 + D\lambda^6 + \frac{E}{\lambda^2} + \frac{\mathrm{F}}{\lambda^4} + \frac{\mathrm{G}}{\lambda^6} + \frac{H}{\lambda^8}$	Extended 2 in Zemax
SCHOTT5X5	$\mathrm{n}(\lambda)^2 = \mathrm{A} + \mathrm{B}\lambda^2 + \mathrm{C}\lambda^4 + D\lambda^6 + E\lambda^8 + \frac{F}{\lambda^2} + \frac{\mathrm{G}}{\lambda^4} + \frac{\mathrm{H}}{\lambda^6} + \frac{J}{\lambda^8} + \frac{K}{\lambda^{10}}$	Extended Schott in TracePro

The general **SELLMEIER** equation looks like:

$$n(\lambda)^2 - 1 = \sum_i \frac{A_i \lambda^2}{\lambda^2 - \lambda_i^2}$$

where λ_i is a wavelength corresponding to an absorption edge. The simplest is a single-term with one wavelength constant. The constant B in the denominator represent an absorption edge wavelengths, usually in the ultraviolet.

Higher-order Sellmeier equations add more terms; as many as four are commonly used and five have been seen. The two-term Sellmeier equation adds an infrared wavelength constant D. Higher order terms are refinements to allow for "soft" edges.

EQN NAME	EQUATION	NOTES
SELL1T	$n(\lambda)^2 - 1 = \frac{A\lambda^2}{\lambda^2 - B^2}$	
SELL2T	$n(\lambda)^2 - 1 = \frac{A\lambda^2}{\lambda^2 - B^2} + \frac{C\lambda^2}{\lambda^2 - D^2}$	ZEMAX, OSLO and TFCalc
SELL3T	$n(\lambda)^2 - 1 = \frac{A\lambda^2}{\lambda^2 - B^2} + \frac{C\lambda^2}{\lambda^2 - D^2} + \frac{E\lambda^2}{\lambda^2 - F^2}$	<u>Sellmeier 1</u> in ZEMAX; also in OSLO, Optalix, TracePro, Sellmeier 3 in TFCalc, Opticad, Schott glass catalog, Laikin 1
SELL4T	$n(\lambda)^2 - 1 = \frac{A\lambda^2}{\lambda^2 - B^2} + \frac{C\lambda^2}{\lambda^2 - D^2} + \frac{E\lambda^2}{\lambda^2 - F^2} + \frac{G\lambda^2}{\lambda^2 - H^2}$	<u>Sellmeier 3</u> in TracePro
SELL5T	$n(\lambda)^2 - 1 = \frac{A\lambda^2}{\lambda^2 - B^2} + \frac{C\lambda^2}{\lambda^2 - D^2} + \frac{E\lambda^2}{\lambda^2 - F^2} + \frac{G\lambda^2}{\lambda^2 - H^2} + \frac{J\lambda^2}{\lambda^2 - K^2}$	Sellmeier 5 in Zemax

CAUTION

Some authors use a linear term (e.g., A) in the denominator of the Sellmeier terms, and others use a squared term (e.g., A^2). The term "A" carries the dimension of wavelength and represents the wavelength of a resonance. Occasionally, negative signs are seen between the Sellmeier terms. Neither are fundamentally flawed, but the signs and magnitudes must be carefully chosen as seeds for most Levenberg-Marquardt non-linear curve-fitting routines.

The most obvious enhancement to the basic Sellmeier equation is to add a constant term to replace the 1.

EQN NAME	EQUATION	NOTES
SELL1TA	$n(\lambda)^2 = A + \frac{B\lambda^2}{\lambda^2 - C^2}$	Sellmeier 1 in TFCalc
SELL2TA	$n(\lambda)^2 = A + \frac{B\lambda^2}{\lambda^2 - C^2} + \frac{D\lambda^2}{\lambda^2 - E^2}$	Sellmeier 4 in ZEMAX and TracePro; Sellmeier 2 in TFCalc; Ghosh ($C=C^2$, $E=E^2$)
SELL3TA	$n(\lambda)^2 = A + \frac{B\lambda^2}{\lambda^2 - C^2} + \frac{D\lambda^2}{\lambda^2 - E^2} + \frac{F\lambda^2}{\lambda^2 - G^2}$	
SELL4TA	$n(\lambda)^2 = A + \frac{B\lambda^2}{\lambda^2 - C^2} + \frac{D\lambda^2}{\lambda^2 - E^2} + \frac{F\lambda^2}{\lambda^2 - G^2} + \frac{H\lambda^2}{\lambda^2 - J^2}$	KCl in HoOII
SELL5TA	$n(\lambda)^2 = A + \frac{B\lambda^2}{\lambda^2 - C^2} + \frac{D\lambda^2}{\lambda^2 - E^2} + \frac{F\lambda^2}{\lambda^2 - G^2} + \frac{H\lambda^2}{\lambda^2 - J^2} + \frac{K\lambda^2}{\lambda^2 - M^2}$	KBr in HoOII
SELL6TA	$n(\lambda)^2 = A + \frac{B\lambda^2}{\lambda^2 - C^2} + \frac{D\lambda^2}{\lambda^2 - E^2} + \frac{F\lambda^2}{\lambda^2 - G^2} + \frac{H\lambda^2}{\lambda^2 - J^2} + \frac{K\lambda^2}{\lambda^2 - M^2} + \frac{N\lambda^2}{\lambda^2 - P^2}$	KI in HoOII
SELL7TA	$n(\lambda)^2 = A + \frac{B\lambda^2}{\lambda^2 - C^2} + \frac{D\lambda^2}{\lambda^2 - E^2} + \frac{F\lambda^2}{\lambda^2 - G^2} + \frac{H\lambda^2}{\lambda^2 - J^2} + \frac{K\lambda^2}{\lambda^2 - M^2} + \frac{N\lambda^2}{\lambda^2 - P^2} + \frac{Q\lambda^2}{\lambda^2 - R^2}$	nAcL in HoOII

Other modifications on the basic and enhanced Sellmeier equations are also found. These are hybrid equations, combinations of the Sellmeier equation with added terms characteristic of the Schott or Herzberger equations. Several examples are shown below:

EQN NAME	EQUATION	NOTES
HoO1	$n(\lambda)^2 = A + B\lambda^2 + \frac{C}{\lambda^2 - D^2}$	Handbook of Optics 1 in ZEMAX, TracePro
HoO2	$n(\lambda)^2 = A + B\lambda^2 + \frac{C\lambda^2}{\lambda^2 - D^2}$	Handbook of Optics 2 in ZEMAX & TracePro; Sellmeier 2' in TFCalc

EQN NAME	EQUATION	NOTES
SELLMOD1	$n(\lambda)^2 = A + B\lambda + C\lambda^2 + \frac{D\lambda^2}{\lambda^2 - E^2}$	
SELLMOD1A	$n(\lambda)^2 = A + B\lambda + C\lambda^2 + \frac{D}{\lambda^2 - E^2}$	
SELLMOD2	$n(\lambda)^2 = A + B\lambda^2 + C\lambda^4 + \frac{D\lambda^2}{\lambda^2 - E^2}$	
SELLMOD2A	$n(\lambda)^2 = A + B\lambda^2 + C\lambda^4 + \frac{D}{\lambda^2 - E^2}$	
SELLMOD3	$n(\lambda)^2 = \frac{A\lambda^2 + B}{\lambda^2 - C^2} + \frac{D\lambda^2}{\lambda^2 - E^2}$	ADP, KDP
SELLMOD4	$n(\lambda)^2 = A + B\lambda^2 + \frac{C}{\lambda^2} + \frac{D\lambda^2}{\lambda^2 - E^2} + \frac{F\lambda^2}{\lambda^2 - G^2}$	
SELLMOD4A	$n(\lambda)^2 = A + B\lambda^2 + \frac{C}{\lambda^2} + \frac{D}{\lambda^2 - E^2} + \frac{F}{\lambda^2 - G^2}$	KBr
SELLMOD5	$n(\lambda)^2 = A + B\lambda^2 + \frac{C\lambda^2}{\lambda^2 - D^2} + \frac{E\lambda^2}{\lambda^2 - F^2}$	$KNbO_3$ in HoOII
SELLMOD6	$n(\lambda)^2 = A + \frac{B\lambda^2}{\lambda^2 - C^2} + \frac{D}{\lambda^2 - E^2}$	Sellmeier 2 in ZEMAX, TracePro and Opticad
SELLMOD7	$n(\lambda)^2 = A + B\lambda^2 + C\lambda^4 + \frac{D}{\lambda^6} + \frac{E\lambda^2}{\lambda^2 - F^2}$	
SELLMOD7A	$n(\lambda)^2 = A + B\lambda^2 + C\lambda^4 + \frac{D}{\lambda^6} + \frac{E}{\lambda^2 - F^2}$	
SELLMOD8	$n(\lambda)^2 = A + B\lambda^2 + C\lambda^4 + \frac{D}{\lambda^2 - E^2} + \frac{F}{\lambda^2 - G^2}$	
SELLMOD9	$n(\lambda)^2 = A + \frac{B}{\lambda^2} + \frac{C}{\lambda^4} + \frac{D}{\lambda^6} + \frac{E\lambda^2}{\lambda^2 - F^2}$	

EQN NAME	EQUATION	NOTES
KINGSLAKE	$n(\lambda)^2 = A + \frac{B}{\lambda^2 - C^2} + \frac{D}{\lambda^2 - E^2} + \cdots$	General form
KINGSLAKE1	$n(\lambda)^2 = A + \frac{B}{\lambda^2 - C^2} + \frac{D}{\lambda^2 - E^2}$	Smith calls this Kettler-Drude, others call it Helmholzz- Drude. used by Li for ZnS & ZnSe
KINGSLAKE2	$n(\lambda)^2 = A + \frac{B}{\lambda^2 - C^2} + \frac{D}{\lambda^2 - E^2} + \frac{F}{\lambda^2 - G^2}$	
MISC01	$n(\lambda)^2 = A + \frac{B}{\lambda^2 - C^2}$	TiO_2 in HoOII
MISC02	$n(\lambda)^2 = A + B\lambda^2 + \frac{C}{\lambda^2 - D^2}$	HoOII(Ag^3AsS_3) HoO
MISC03	$n(\lambda)^2 = A + \frac{B}{\lambda^2} + \frac{C\lambda^2}{\lambda^2 - D^2}$	CuCl in HoOII
MISC04	$n(\lambda)^2 = A + B\lambda^2 + C\lambda^4 + \frac{D}{\lambda^2} + \frac{E\lambda^2}{\lambda^2 - F + \left[G\lambda^2/\left(\lambda^2 - F\right)\right]}$	Bausch and Lomb
MISC05	$n(\lambda)^2 = A + \frac{B/\lambda^2}{1 - \lambda^2/C} + \frac{D}{E - 1/\lambda^2}$	JOSA 54, 1215

NOTE: The **EQN NAME** column identifies a **.EQN** equation file used in PSI-Plot. I use this program for non-linear regression curve fitting using the Levenberg-Marquardt algorithm.

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