Appendix C

Multivariable regression for the synchrotron losses fit

As seen in Chapter 3, the transparency factor parameter Φ^* in an inhomogeneous plasma torus only depends explicitly on the dimensionless parameter p_a and R. The geometrical dimensionless parameters A and κ participate in the calculation of the ray path length, in the plasma surface integration, and in the $R(\sigma)$ calculation (see Eq. (3.58)), also affecting implicitly to the plasma self-absorption. As for the central density and magnetic field (gathered inside the parameter p_a), central temperature, and shape of profiles, they take part in the calculation of the absorption coefficients. Consequently, a priori we cannot suggest neither simple relationships between fitting variables nor direct dependences of Φ^* with such variables.

C.1 The best monomial fit

First, we propose a monomial model with the fitting variables T_{e_0}, p_{a_0}, κ, α_n, α_T, β_T as

$$\Phi^*_{\text{fit}} = C_{\Phi^*} T_{e_0}^{x_T}\, p_{a_0}^{x_p}\, \kappa^{x_\kappa}\, (C_{\alpha_n} + \alpha_n)^{x_{\alpha_n}}\, (C_{\alpha_T} + \alpha_T)^{x_{\alpha_T}}\, \beta_T^{x_{\beta_T}} \tag{C.1}$$

in order to fit the numerical results from the complete computation of synchrotron losses in toroidal plasmas with an aspect ratio $A = 3$. In this case, we have the following $p = 9$ parameters to be estimated: C_{Φ^*}, x_T, x_p, x_κ, x_{α_n}, x_{α_T}, x_{β_T}, C_{α_n} and C_{α_T}[1].

Note that this model is intrinsically linear in the above parameters by transfor-

[1]The fit parameters are those resulting from the regression whilst the fitting variables are the physical plasma parameters which act as the input regression data.

mation of the variables. Indeed, taking natural logarithms of both sides we obtain

$$\begin{aligned}\ln \Phi^*_{\text{fit}} = \ln C_{\Phi^*} + x_T T_{e_0} + x_p p_{a_0} + x_\kappa \kappa + x_{\alpha_n} \left(C_{\alpha_n} + \alpha_n\right) \\ + x_{\alpha_T} \left(C_{\alpha_T} + \alpha_T\right) + x_{\beta_T} \beta_T,\end{aligned} \tag{C.2}$$

where the fit parameters are adjusted to achieve a minimum in the least-squares merit function F, which gives the name to this regression method. Defining the residual ε_i as the difference between the transformed value of the complete numerical calculation of the transparence factor $\Phi^*_{\text{num}_i}$ for the i set of data and the values predicted by the logarithmic regression model for the same set of data, F is the sum of squares of residuals for the entire dataset with $A = 3$. For n_{data} set of data points,

$$F = \sum_{i=1}^{n} \varepsilon_i^2 = \sum_{i=1}^{n_{\text{data}}} \left(\ln \Phi^*_{\text{num}_i} - \ln \Phi^*_{\text{fit}_i}\right)^2$$

i.e.,

$$F = \sum_{i=1}^{n_{\text{data}}} \ln^2 \frac{\Phi^*_{\text{num}_i}}{\exp\left[\ln C_{\Phi^*} + x_T T_{e_0} + x_p p_{a_0} + x_\kappa \kappa + x_{\alpha_n}(C_{\alpha_n} + \alpha_n) + x_{\alpha_T}\left(C_{\alpha_T} + \alpha_T\right) + x_{\beta_T}\beta_T\right]}. \tag{C.3}$$

Note that minimizing the least-square function is a maximum likelihood estimation of the fit parameters whenever the errors of the complete computation of the factor Φ^* are independent and normally distributed with a constant standard deviation. Let us check now the latter condition. The computation of the factor Φ^*_i is performed numerically with a requested relative error of $e_{\text{rel},i} = 2 \times 10^{-2}$ for the entire dataset with $A = 3$. The standard deviation $\sigma_{\text{num},i}$ of such a computation is derived from $e_{\text{rel},i}$ by means of

$$\sigma_{\text{num}_i} \propto \left|\overline{\Phi^*}_i - \Phi^*_{\text{num}_i}\right| = e_{\text{rel},i}\, \Phi^*_{\text{num}_i},$$

where $\overline{\Phi^*}_i$ is the true result of Eq. (3.59). Transforming variables in logarithms, we obtain a constant transformed standard deviation of the complete numerical calculation of the factor Φ^* for any set i of data points,

$$\sigma_{\text{num(log)}_i} \propto \left|\ln \overline{\Phi^*}_i - \ln \Phi^*_{\text{num}_i}\right| = \ln\left(1 + e_{\text{rel},i}\right)$$

Therefore, the errors of the numerical calculation of Φ^* are normally distributed and the least-squared method for fitting the logarithmic monomial model is fully justified.

Considering the entire dataset with $A = 3$, Eq. (C.2) can be expressed in matrix notation as follows [Dra81]:

$$\boldsymbol{Y} = \boldsymbol{X}\, \boldsymbol{b} + \boldsymbol{\varepsilon}$$

with

$$\boldsymbol{Y}=\begin{bmatrix} \ln \Phi^*_{\text{num}_1} \\ \cdots \\ \ln \Phi^*_{\text{num}_i} \\ \cdots \\ \ln \Phi^*_{\text{num}_{n_{\text{data}}}} \end{bmatrix}, \quad \boldsymbol{b}=\begin{bmatrix} \ln C_{\Phi^*} \\ x_T \\ x_p \\ x_\kappa \\ x_{\alpha_n} \\ x_{\alpha_T} \\ x_{\beta_T} \end{bmatrix},$$

$$\boldsymbol{X}=\begin{bmatrix} 1 & T_{e_{0,1}} & p_{a_{0,1}} & \kappa_1 & C_{\alpha_n}+\alpha_{n_1} & C_{\alpha_T}+\alpha_{T_1} & \beta_{T_1} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 1 & T_{e_{0,i}} & p_{a_{0,i}} & \kappa_i & C_{\alpha_n}+\alpha_{n_i} & C_{\alpha_T}+\alpha_{T_i} & \beta_{T_i} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 1 & T_{e_{0,n_{\text{data}}}} & p_{a_{0,n_{\text{data}}}} & \kappa_{n_{\text{data}}} & C_{\alpha_n}+\alpha_{n_{n_{\text{data}}}} & C_{\alpha_T}+\alpha_{T_{n_{\text{data}}}} & \beta_{T_{n_{\text{data}}}} \end{bmatrix},$$

and $\boldsymbol{\varepsilon}$ is the vector of residuals.

The minimization of the merit function F to $\ln C_{\Phi^*}$ and exponent parameters

$$\frac{\partial F}{\partial \ln C_{\Phi^*}}=0, \quad \frac{\partial F}{\partial x_T}=0, \quad \frac{\partial F}{\partial x_p}=0, \quad \frac{\partial F}{\partial x_\kappa}=0,$$
$$\frac{\partial F}{\partial x_{\alpha_n}}=0, \quad \frac{\partial F}{\partial x_{\alpha_T}}=0, \quad \frac{\partial F}{\partial x_{\beta_T}}=0$$

can be also written as

$$\boldsymbol{b}=\left(\boldsymbol{X}'\boldsymbol{X}\right)^{-1}\boldsymbol{X}'\boldsymbol{Y}$$

with a variance estimated by

$$V\left(\boldsymbol{b}\right)=\left(\boldsymbol{X}'\boldsymbol{X}\right)^{-1}\sigma^2_{\text{num(log)}}.$$

The rest of parameters (C_{α_n} and C_{α_T}) are derived from the minimization of the residual ε_i mean square, which is defined as

$$s^2_\varepsilon=\frac{\sum_{i=1}^{n_{\text{data}}}\left(\varepsilon_i-\overline{\varepsilon}\right)^2}{n_{\text{data}}-7}.$$

As a property of the regression residuals, it is found that $\overline{\varepsilon}=0$. Hence, it can also be written that $s^2_\varepsilon=F/\left(n_{\text{data}}-p-2\right)$. The residual root mean square, which is denoted as root mean square error (RMSE), is then

$$\text{RMSE}=\sqrt{\frac{F}{n_{\text{data}}-7}}$$

and it provides an estimate of the variance about the regression based on $n_{\text{data}}-7$ degrees of freedom. The RMSE can be expressed on a percentage basis, since in the merit function F, in Eq. (C.3), the factor $\Phi^*_{\text{num}_i}$ is normalized to $\Phi^*_{\text{fit}_i}$.

Table C.1: Fit parameters minimizing the merit function F of the multidimensional least-squares method using a power law model, with the corresponding σ confidence region.

Parameter	best fitting $\pm$ σ
$\ln C_\Phi$	-5.540 ± 0.023
x_T	1.445 ± 0.004
x_p	-0.477 ± 0.003
x_κ	0.794 ± 0.006
x_{α_n}	-0.426 ± 0.020
x_{α_T}	-0.329 ± 0.003
x_{β_T}	0.454 ± 0.004
C_{α_n}	1.50 ± 0.05
C_{α_T}	0.10 ± 0.05

C.1.1 Results and examination of residuals

Applying the multidimensional linear method described above using $n_{\text{data}} = 2475$ set of plasma parameters and computations of the factor Φ^*, we obtain the fit parameters presented in Table C.1 with a poor RMSE equal to 27%.

Fig. 3.24 compares the distribution of residuals with a normal distribution of standard deviation $\sigma =$ RMSE. On the ordinate of this graph, we have the number of residuals n_{ε_i} whose values are within the interval $\varepsilon_i \pm \Delta H/2$ normalized both to the box width ΔH and to the total number of data n_{data}. We see that the distribution of residuals do not resemble to a normal distribution. Moreover, Fig. C.2 shows that there are cross-dependencies between fitting variables that are not taken into account in Eq. (C.1). We therefore conclude that such a monomial regression model is not adequate to explain the factor plasma transparency factor Φ^*.

The analysis of residuals show also that the variables introducing the largest uncertainty in this model are the temperature peaking coefficients α_T, β_T. This means that the dependence of such coefficients on synchrotron losses is not well described by the monomial form.

C.2 Addition of interaction terms to the regression model

We suggest a method for isolating the variables which interacts in their effect on the response Φ^*. This approach consists of analysing the dependence of each plasma variable ($T_{e_0}, p_a, \kappa, \alpha_n, \beta_T, \alpha_T$) on each exponent fit parameter (x_T, x_p, x_κ, x_{α_n}, x_{α_T}, x_{β_T}), using the monomial model (Eq. (C.1)).

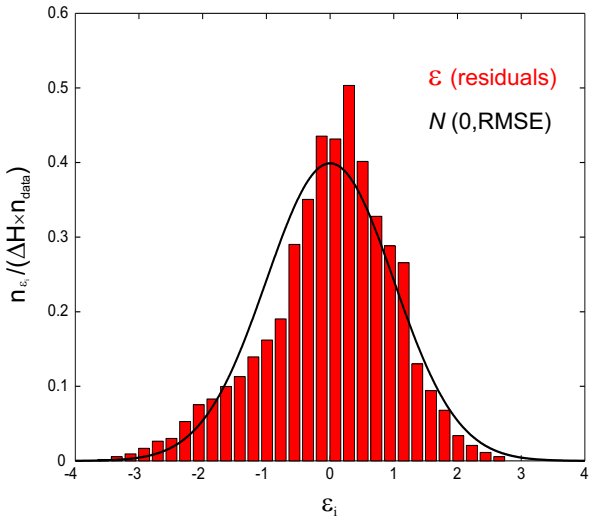

Figure C.1: Distribution of regression residuals represented by red boxes, and the normal distribution $N\,(0, \mathrm{RMSE})$ represented by the black curve.

For one value of a given plasma variable (e.g. $\alpha_T = 0$), the best exponent parameters are found (e.g. $x_t = 1.44$) by applying the multidimensional linear method to the part of the dataset corresponding to such a variable value. Next this process is repeated four times for other values of the same variable (e.g. $\alpha_T = 0.3$, 0.9, 2.7, 8), obtaining a set of parameters for each exponent, and the root mean square for each set s_{x_j} is calculated. The schematic results of this approach performed for every plasma variable are shown in Table C.2, where $\surd$ means a strong dependence ($s_{x_j} > 0.1$), ✓ means a substantial dependence ($5 \times 10^{-2} < s_{x_j} < 0.1$), $\backsim$ means a marginal dependence ($1 \times 10^{-3} < s_{x_j} < 5 \times 10^{-2}$), and – means no dependence observed ($s_{x_j} < 1 \times 10^{-3}$).

Table C.2: Schematic variance of the exponent parameters with the plasma fitting variables ($*$ means not applicable).

	T_{e_0}	p_{a_0}	κ	α_n	α_T	β_T
x_t	$*$	✓	–	$\backsim$	$\surd$	–
x_p	✓	$*$	–	$\backsim$	–	–
x_κ	–	–	$*$	–	–	–
x_{α_n}	$\backsim$	$\backsim$	–	$*$	$\surd$	$\backsim$
x_{α_T}	$\backsim$	–	–	✓	$*$	$\surd$
x_{β_T}	✓	–	–	✓	$\surd$	$*$

From Table C.2 the following main relationships are suggested: temperature

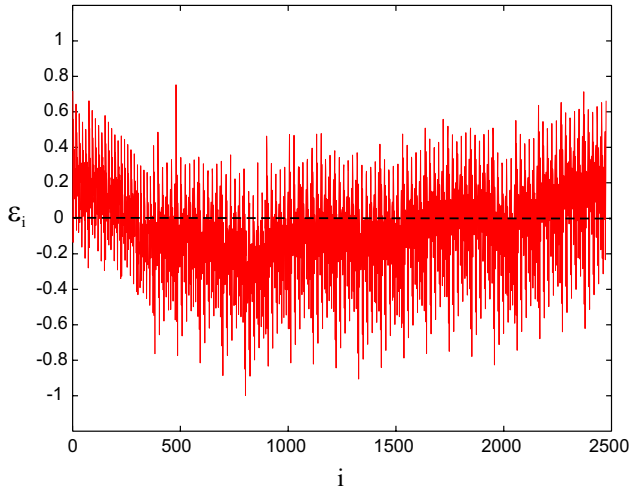

Figure C.2: Residuals $\varepsilon_i = \ln\left(\Phi^*_{\text{num}_i}/\Phi^*_{\text{fit}_i}\right)$ plotted in time order ι.

peaking coefficients α_T, β_T are strongly interdependent and the temperature and opacity factor T_{e_0}, p_{a_0}, as well as the α_n, α_T peaking coefficients, interact reciprocally on Φ^*. This confirms the results obtained in the analysis of residuals of Φ^* modelled with a simple monomial model.

C.2.1 The multidimensional weighted least-squares method

A no longer intrinsically linear model is considered in order to include interactions between variables and therefore to obtain a more convenient fitting goodness. Here, the variables are not transformed, and the standard deviation $\sigma_{\text{num},i}$ of the complete computation of $\Phi^*_{\text{num},i}$ will be different for every set of data[2],

$$\sigma_{\text{num},i} \propto e_{\text{rel},i}\, \Phi^*_{\text{num},i}.$$

Consequently, the maximum likelihood estimate of the fit parameters is obtained by minimizing the merit function F (the sum of squares of residuals for the entire dataset with $A = 3$) weighted with its numerical standard deviation:

$$F = \sum_{i=1}^{n_{\text{data}}} \left(\frac{\Phi^*_{\text{num},i} - \Phi^*_{\text{fit},i}}{\sigma_{\text{num},i}} \right)^2 \propto \sum_{i=1}^{n_{\text{data}}} \left(1 - \frac{\Phi^*_{\text{fit},i}}{\Phi^*_{\text{num},i}} \right)^2 .$$

Let us notice that, in this case, minimizing the merit function is equivalent to minimizing the sum of squares of the relative difference between the predicted value $\Phi^*_{\text{fit},i}$ and the numerical one $\Phi^*_{\text{num},i}$.

[2]The numerical deviations $\left|\overline{\Phi^*}_i - \Phi^*_{\text{num}_i}\right|$ are assumed to be uncorrelated.

For a regression model with p fit parameters, the residual mean square is expressed as

$$s_\varepsilon^2 = \frac{\sum_{i=1}^{n_{\text{data}}} \varepsilon_i^2}{n_{\text{data}} - p} = \frac{F}{n_{\text{data}} - p},$$

where the residuals ε_i to be examined are

$$\varepsilon_i = \left(1 - \frac{\Phi^*_{\text{fit},i}}{\Phi^*_{\text{num},i}}\right).$$

The RMSE indicator is the root of s_ε^2 (RMSE$= \sqrt{F/\left(n_{\text{data}} - p\right)}$) and it is currently expressed on a percentage basis.

C.2.2 Selection of the regression model

Using Table C.2 and the multidimensional weighted least-squares method described above, an exhaustive analysis for selecting the best regression model for Φ^*, including cross-dependences between fitting variables, has been carried out. In Table C.3 we illustrate the increase of the regression quality when including new terms. Note that although many other forms of dependence have been tested, we only show those which make to improve the regression quality:

Cross-dependence between α_T, β_T

$$\Phi^*_{\text{fit}} = C_{\Phi^*} T_{e_0}^{x_T}\, p_{a_0}^{x_p}\, \kappa^{x_\kappa}\, \left(C_{\alpha_n} + \alpha_n\right)^{x_{\alpha_n}} \left(C_{\alpha\beta} + C_{\alpha_T}\alpha_T^{x_{\alpha_T}} + \beta_T^{x_{\beta_T}}\right) \tag{C.4}$$

$$\begin{aligned}\Phi^*_{\text{fit}} = {} & C_{\Phi^*} T_{e_0}^{x_T}\, p_{a_0}^{x_p}\, \kappa^{x_\kappa}\, \left(C_{\alpha_n} + \alpha_n\right)^{x_{\alpha_n}} \\ & \times \left(C_{\alpha_T} + \alpha_T\right)^{x_{\alpha_T}}\, \beta_T^{x_{\beta_T}}\, \left(C_{\alpha_1}\alpha_T + \beta_T\right)^{x_{\alpha\beta}}\end{aligned} \tag{C.5}$$

$$\begin{aligned}\Phi^*_{\text{fit}} = {} & C_{\Phi^*} T_{e_0}^{x_T}\, p_{a_0}^{x_p}\, \kappa^{x_\kappa}\, \left(C_{\alpha_n} + \alpha_n\right)^{x_{\alpha_n}} \\ & \times \left(C_{\alpha_T} + \alpha_T\right)^{x_{\alpha_T}}\, \beta_T^{x_{\beta_1}}\, \left(\beta_T^{x_{\beta 2}} + C_{\alpha_1}\alpha_T + C_{\alpha\beta}\right)^{x_{\alpha\beta}}\end{aligned} \tag{C.6}$$

Cross-dependence between α_n, α_T (and β_T)

$$\begin{aligned}\Phi^*_{\text{fit}} = {} & C_{\Phi^*} T_{e_0}^{x_T}\, p_{a_0}^{x_p}\, \kappa^{x_\kappa}\, \left[\left(C_{\alpha_n} + \alpha_n\right)^{x_{\alpha_n}} + C_{\alpha_3}\alpha_T + C_\beta\beta_T + C_{\alpha_2}\right]^{x_\alpha} \\ & \times \left(C_{\alpha_T} + \alpha_T\right)^{x_{\alpha_T}}\, \beta_T^{x_{\beta 1}}\, \left(\beta_T^{x_{\beta 2}} + C_{\alpha_1}\alpha_T + C_{\alpha\beta}\right)^{x_{\alpha\beta}}\end{aligned} \tag{C.7}$$

$$\begin{aligned}\Phi^*_{\text{fit}} = {} & C_{\Phi^*} T_{e_0}^{x_T}\, p_{a_0}^{x_p}\, \kappa^{x_\kappa}\, \left(\alpha_n + C_{\alpha_2}\alpha_T + C_{\alpha_n}\right)^{x_{\alpha_n}} \\ & \times \left(C_{\alpha_T} + \alpha_T\right)^{x_{\alpha_T}}\, \beta_T^{x_{\beta_1}}\, \left(\beta_T^{x_{\beta 2}} + C_{\alpha_1}\alpha_T + C_{\alpha\beta}\right)^{x_{\alpha\beta}}\end{aligned} \tag{C.8}$$

Cross-dependence between T_{e_0}, p_{a_0}

$$\begin{aligned}\Phi^*_{\text{fit}} = {} & C_{\Phi^*}\left(C_T + T_{e_0}\right)^{x_T} p_{a_0}^{x_p}\, \kappa^{x_\kappa}\left(\alpha_n + C_{\alpha_2}\alpha_T + C_{\alpha_n}\right)^{x_{\alpha_n}} \\ & \times \left(C_{\alpha_T} + \alpha_T\right)^{x_{\alpha_T}} \beta_T^{x_{\beta_1}} \left(\beta_T^{x_{\beta 2}} + C_{\alpha_1}\alpha_T + C_{\alpha\beta}\right)^{x_{\alpha\beta}}\end{aligned} \tag{C.9}$$

$$\begin{aligned}\Phi^*_{\text{fit}} = {} & C_{\Phi^*}\left(C_T + T_{e_0}\right)^{x_T} \left(C_{pT} + p_{a_0}^{x_p} + C_p T_{e_0}\right)^{x_{pT}}\, \kappa^{x_\kappa}\left(\alpha_n + C_{\alpha_2}\alpha_T + C_{\alpha_n}\right)^{x_{\alpha_n}} \\ & \times \left(C_{\alpha_T} + \alpha_T\right)^{x_{\alpha_T}} \beta_T^{x_{\beta_1}} \left(C_{\alpha\beta} + C_{\alpha_1}\alpha_T + \beta_T^{x_{\beta_2}}\right)^{x_{\alpha\beta}}\end{aligned} \tag{C.10}$$

$$\begin{aligned}\Phi^*_{\text{fit}} = {} & C_{\Phi^*}\left(C_T + T_{e_0}\right)^{x_T} \left(p_{a_0}^{x_p} + C_p T_{e_0}\right)^{x_{pT}}\, \kappa^{x_\kappa}\left(\alpha_n + C_{\alpha_2}\alpha_T + C_{\alpha_n}\right)^{x_{\alpha_n}} \\ & \times \left(C_{\alpha_T} + \alpha_T\right)^{x_{\alpha_T}} \beta_T^{x_{\beta_1}} \left(\beta_T^{x_{\beta 2}} + C_{\alpha_1}\alpha_T + C_{\alpha\beta}\right)^{x_{\alpha\beta}}\end{aligned} \tag{C.11}$$

Cross-dependence between p_{a_0}, α_n

$$\begin{aligned}\Phi^*_{\text{fit}} = {} & C_{\Phi^*}\left(C_T + T_{e_0}\right)^{x_T} \left(p_{a_0}^{x_p} + C_p T_{e_0}\right)^{x_{pT}}\, \kappa^{x_\kappa} \\ & \times \left(C_{p_2} p_{a_0}^{x_{p2}} + \alpha_n + C_{p\alpha}\right)^{x_{p\alpha}} \left(\alpha_n + C_{\alpha_2}\alpha_T + C_{\alpha_n}\right)^{x_{\alpha_n}} \\ & \times \left(C_{\alpha_T} + \alpha_T\right)^{x_{\alpha_T}} \beta_T^{x_{\beta_1}} \left(\beta_T^{x_{\beta 2}} + C_{\alpha_1}\alpha_T + C_{\alpha\beta}\right)^{x_{\alpha\beta}}\end{aligned} \tag{C.12}$$

Table C.3: Goodness of several models taking into account the main cross-dependences between the fitting variables, where p is the number of parameters.

Model	p	RMSE (%)
Eq. (C.1)	9	28.7
Eq. (C.4)	10	17.9
Eq. (C.5)	11	14.3
Eq. (C.6)	13	13.4
Eq. (C.7)	17	11.1
Eq. (C.8)	14	10.9
Eq. (C.9)	15	7.9
Eq. (C.10)	18	5.8
Eq. (C.11)	17	5.8
Eq. (C.12)	21	5.5

In Table C.3 we observe a substantial improvement of the regression quality when including the cross-dependence between α_n, β_T (from RMSE $\simeq$ 29% to 13%. The cross-dependences between α_n**,** α_T and between T_{e_0}**,** p_{a_0} reduce the RMSE up to 5.8%. Finally, the RMSE is slightly reduced by 0.3% when including the cross-dependence between p_{a_0}**,** α_n, but at the expense of increasing by 4 the number of the model parameters. On account of these elements, Eq. (C.11) has been proposed as the regression model for fitting synchrotron losses. It takes into account the cross-dependences between α_T and β_T, α_n and α_T, T_{e_0} and p_{a_0}, with a number of parameters $p = 16$.

In Table C.4 we show the resulting parameters minimizing the merit function F for the selected model. Note that in this non-linear case, the confidence region for each parameter $(\pm\sigma)$ is estimated by linearizing Eq. (C.11), as discussed in Ref. [Dra81].

Table C.4: Fit parameters minimizing the merit function F of the multidimensional weighted least-squares method using Eq. (C.11), with the corresponding σ confidence region.

Parameter	best fitting $\pm$ σ
C_{Φ^*}	$6.86 \times 10^{-5} \pm 3 \times 10^{-6}$
x_T	2.61 ± 0.04
C_T	16.0 ± 0.38
x_{pT}	-1.51 ± 0.08
x_p	0.41 ± 0.02
C_p	0.12 ± 0.02
x_κ	0.79 ± 0.04
x_{α_n}	-0.79 ± 0.06
C_{α_2}	3.87 ± 0.27
C_{α_n}	1.46 ± 0.17
x_{α_T}	1.36 ± 0.05
C_{α_T}	1.98 ± 0.15
x_{β_1}	2.14 ± 0.04
$x_{\alpha\beta}$	-1.33 ± 0.03
x_{β_2}	1.53 ± 0.02
C_{α_1}	1.87 ± 0.07
$C_{\alpha\beta}$	-0.16 ± 0.01

The distribution of residuals and the final form of the fit are presented in Chapter 3.