

# On the vapour pressure over three-component solutions

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## Abstract

The work [1] describes equations relating the dependence of the partial vapour pressures of components above a binary solution on its composition with the Henry constants and the second virial coefficients of the solution.

An attempt has been made to generalize these equations to three-component solutions.

In [1], equations were derived that connect the dependence of the partial vapour pressures of components above a binary solution on its composition with Henry's constants and second virial coefficients:

$$\frac{P_x}{P_x^o} = xe^{f(y)}; \quad \frac{P_y}{P_y^o} = ye^{\varphi(x)} \quad (1)$$

Here  $P_x$  and  $P_y$  are the partial vapour pressures of the first and second components above their binary solution,  $P_x^o$  and  $P_y^o$  are the vapour pressures above the corresponding pure components,  $x$  and  $y$  are their mole fractions in the solution ( $x + y = 1$ ) and

$$\begin{cases} f(y) = \alpha y^2 + (12B - 8A + 2\beta - 6\alpha)y^3 + (21A - 24B + 9\alpha - 6\beta)y^4 + (12B - 12A + 4\beta - 4\alpha)y^5 \\ \varphi(x) = \beta x^2 + (12A - 8B + 2\alpha - 6\beta)x^3 + (21B - 24A + 9\beta - 6\alpha)x^4 + (12A - 12B + 4\alpha - 4\beta)x^5 \end{cases} \quad (2)$$

wherein the parameters  $A, B, \alpha$  and  $\beta$  are related to the Henry constants and the second virial coefficients of the solution as follows [1]:

$$A = \ln\left(\frac{K_x}{P_x^o}\right); \quad B = \ln\left(\frac{K_y}{P_y^o}\right); \quad \alpha = \frac{W_x}{V_x^o}; \quad \beta = \frac{W_y}{V_y^o}, \quad (3)$$

where  $K_x$  and  $K_y$  are Henry's constants,  $W_x$  and  $W_y$  are the second virial coefficients,  $V_x^o$  and  $V_y^o$  are the molar volumes of pure components.

The purpose of this work is to generalize these formulas (1–2) to three-component solutions. This would make it possible, knowing the behaviour of three binary solutions composed in pairs from the components of the ternary solution, to predict the behaviour of the ternary solution, including possible areas of unmixing [2].

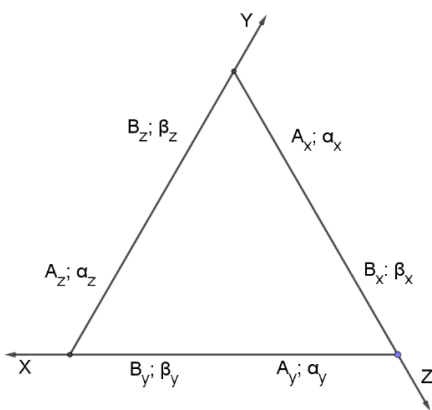


Fig. 1 Roseboom-triangle. Explanations in the text.

Further we use the following notations:  $x, y$  and  $z$  are the mole fractions of the components in a three-component solution ( $x + y + z = 1$ ), and parameters (3) for three binary solutions (XY, YZ and ZX – see Fig. 1) have subscripts indices indicating the absence of the third component (for example,  $A_z$  denotes parameter  $A$  in the absence of component  $Z$ , i.e. for a binary solution XY).

We will look for a solution in a form similar to (1):

$$\frac{P_x}{P_x^o} = xe^{f(y,z)}; \quad \frac{P_y}{P_y^o} = ye^{\varphi(z,x)}; \quad \frac{P_z}{P_z^o} = ze^{\xi(x,y)}, \quad (4)$$

and we will look for functions under exponents (similarly to a binary solution) in the form of 5-degree polynomials of two arguments:

$$f(y, z) = \sum_{i=0}^5 \sum_{j=0}^{5-i} a_{ij} y^i z^j; \quad \varphi(z, x) = \sum_{i=0}^5 \sum_{j=0}^{5-i} b_{ij} z^i x^j; \quad \xi(x, y) = \sum_{i=0}^5 \sum_{j=0}^{5-i} c_{ij} x^i y^j \quad (5)$$

wherein, the coefficients  $a_{ij}$ ,  $b_{ij}$ ,  $c_{ij}$  must be related to the constants  $A_i$ ,  $B_i$ ,  $\alpha_i$  and  $\beta_i$  for three binary solutions.

On the side of the triangle  $z = 0$ , all terms of the polynomial containing  $z$  vanish; it remains:

$$f(y, z = 0) = a_{00} + a_{10}y + a_{20}y^2 + a_{30}y^3 + a_{40}y^4 + a_{50}y^5$$

$$\varphi(z = 0, x) = b_{00} + b_{01}x + b_{02}x^2 + b_{03}x^3 + b_{04}x^4 + b_{05}x^5$$

From comparison with formulas (2) it immediately follows:

$$\begin{aligned} a_{00} &= 0 & b_{00} &= 0 \\ a_{10} &= 0 & b_{01} &= 0 \\ a_{20} &= \alpha_z & b_{02} &= \beta_z \\ a_{30} &= 12B_z - 8A_z + 2\beta_z - 6\alpha_z & b_{03} &= 12A_z - 8B_z + 2\alpha_z - 6\beta_z \\ a_{40} &= 21A_z - 24B_z + 9\alpha_z - 6\beta_z & b_{04} &= 21B_z - 24A_z + 9\beta_z - 6\alpha_z \\ a_{50} &= 12B_z - 12A_z + 4\beta_z - 4\alpha_z & b_{05} &= 12A_z - 12B_z + 4\alpha_z - 4\beta_z \end{aligned} \quad (5)$$

Similarly, from a comparison of the formulas on the side of the triangle  $x = 0$  it follows:

$$\begin{aligned} b_{00} &= 0 & c_{00} &= 0 \\ b_{10} &= 0 & c_{01} &= 0 \\ b_{20} &= \alpha_x & c_{02} &= \beta_x \\ b_{30} &= 12B_x - 8A_x + 2\beta_x - 6\alpha_x & c_{03} &= 12A_x - 8B_x + 2\alpha_x - 6\beta_x \\ b_{40} &= 21A_x - 24B_x + 9\alpha_x - 6\beta_x & c_{04} &= 21B_x - 24A_x + 9\beta_x - 6\alpha_x \\ b_{50} &= 12B_x - 12A_x + 4\beta_x - 4\alpha_x & c_{05} &= 12A_x - 12B_x + 4\alpha_x - 4\beta_x \end{aligned} \quad (6)$$

and on side  $y = 0$  –

$$\begin{aligned} a_{00} &= 0 & c_{00} &= 0 \\ a_{01} &= 0 & c_{10} &= 0 \\ a_{02} &= \beta_y & c_{20} &= \alpha_y \\ a_{03} &= 12A_y - 8B_y + 2\alpha_y - 6\beta_y & c_{30} &= 12B_y - 8A_y + 2\beta_y - 6\alpha_y \\ a_{04} &= 21B_y - 24A_y + 9\beta_y - 6\alpha_y & c_{40} &= 21A_y - 24B_y + 9\alpha_y - 6\beta_y \\ a_{05} &= 12A_y - 12B_y + 4\alpha_y - 4\beta_y & c_{50} &= 12B_y - 12A_y + 4\beta_y - 4\alpha_y \end{aligned} \quad (7)$$

30 parameters remain unknown.

Inside the Roseboom triangle, the functions must satisfy the Duhem–Margules equation:

$$\sum n_i d \ln a_i = 0,$$

where  $a_i$  is the activity of the  $i$ -th component of the solution ( $a_i = P_i/P_i^\circ$ ). Taking into account (4), we obtain:

$\ln a_x = \ln x + f(y, z); \quad \ln a_y = \ln y + \varphi(z, x); \quad \ln a_z = \ln z + \xi(x, y);$  then

$$d \ln a_x = \frac{dx}{x} + \frac{\partial f}{\partial x} dx + \frac{\partial f}{\partial y} dy; \quad d \ln a_y = \frac{dy}{y} + \frac{\partial \varphi}{\partial x} dx + \frac{\partial \varphi}{\partial y} dy; \quad d \ln a_z = -\frac{dx}{z} - \frac{dy}{z} + \frac{\partial \xi}{\partial x} dx + \frac{\partial \xi}{\partial y} dy$$

Substituting the last three formulas into the Duhem–Margules equation leads to the equality:

$$\left( x \frac{\partial f}{\partial x} + y \frac{\partial \varphi}{\partial x} + z \frac{\partial \xi}{\partial x} \right) dx + \left( x \frac{\partial f}{\partial y} + y \frac{\partial \varphi}{\partial y} + z \frac{\partial \xi}{\partial y} \right) dy = 0$$



Substituting functions (5) into equations (8) and taking into account that  $z = 1 - x - y$ , we obtain a system of 30 linear equations for 30 unknown coefficients  $a_{ij}$ ,  $b_{ij}$ ,  $c_{ij}$  (for detailed calculations, see the Appendix); it is tabulated (see Table 1). This table is an expanded matrix of an equations system; the matrix of the left side consists of columns from  $a_{11}$  to  $c_{41}$ , the matrix of the right side – of column from  $A_x$  to  $\beta_z$ . To make the table easier to understand, we explain its meaning using the example of its first line: it means  $b_{11} + b_{21} + b_{31} + b_{41} + c_{11} = 2\beta_x$ .

The system was solved using Excel matrix functions.

Unexpectedly, it turned out that the matrix on the left side is singular (its determinant is equal to zero). At the same time, the right side of the system of equations is not equal to zero. This means that the system is inconsistent.

This result is surprising: the physical meaning of the problem implies that a solution must exist.

Therefore, the announced purpose of this work has not been achieved, and the task has not been solved.

### Literature:

1. Levinsky A.I. "Dependence of partial vapour pressures on the composition of a binary solution" // Russian Journal of Physical Chemistry, 1990, v. 64, p. 1388.
2. Levinsky A.I. Are there binary solutions with two regions of unmixing? // Journal of Physical Chemistry, 2002, v. 76 No. 1, p. 134-135.

## Appendix: mathematical calculations.

From  $z = 1 - x - y$  it follows:

$$\begin{aligned} x \frac{\partial f[y; z(x, y)]}{\partial x} &= x \frac{\partial f}{\partial z} \frac{\partial z}{\partial x} = -x \frac{\partial f}{\partial z} = \\ &= -2a_{02}xz - 3a_{03}xz^2 - 4a_{04}xz^3 - 5a_{05}xz^4 - a_{11}xy - 2a_{12}xyz - 3a_{13}xyz^2 - 4a_{14}xyz^3 - a_{21}xy^2 \\ &\quad - 2a_{22}xy^2z - 3a_{23}xy^2z^2 - a_{31}xy^3 - 2a_{32}xy^3z - a_{41}xy^4 \end{aligned}$$

$$\begin{aligned} y \frac{\partial \varphi[z(x, y); x]}{\partial x} &= y \frac{\partial \varphi}{\partial x} + y \frac{\partial \varphi}{\partial z} \frac{\partial z}{\partial x} = y \frac{\partial \varphi}{\partial x} - y \frac{\partial \varphi}{\partial z} = \\ &= 2b_{02}xy + 3b_{03}x^2y + 4b_{04}x^3y + 5b_{05}x^4y + b_{11}yz + 2b_{12}xyz + 3b_{13}x^2yz + 4b_{14}x^3yz + b_{21}yz^2 \\ &\quad + 2b_{22}xyz^2 + 3b_{23}x^2yz^2 + b_{31}yz^3 + 2b_{32}xyz^3 + b_{41}yz^4 - b_{11}xy - b_{12}x^2y - b_{13}x^3y - b_{14}x^4y \\ &\quad - 2b_{20}yz - 2b_{21}xyz - 2b_{22}x^2yz - 2b_{23}x^3yz - 3b_{30}yz^2 - 3b_{31}xyz^2 - 3b_{32}x^2yz^2 - 4b_{40}yz^3 \\ &\quad - 4b_{41}xyz^3 - 5b_{50}yz^4 \end{aligned}$$

$$\begin{aligned} z \frac{\partial \xi(x; y)}{\partial x} &= \\ &= c_{11}yz + c_{12}y^2z + c_{13}y^3z + c_{14}y^4z + 2c_{20}xz + 2c_{21}xyz + 2c_{22}xy^2z + 2c_{23}xy^3z + 3c_{30}x^2z \\ &\quad + 3c_{31}x^2yz + 3c_{32}x^2y^2z + 4c_{40}x^3z + 4c_{41}x^3yz + 5c_{50}x^4z \end{aligned}$$

We replace  $z$  with  $(1 - x - y)$ , dissolve the brackets and combine the similar terms:

$$\begin{aligned} x \frac{\partial f}{\partial x} &= \\ &= -2a_{02}x(1 - x - y) - 3a_{03}x(1 - 2y + y^2 - 2x + 2xy + x^2) \\ &\quad - 4a_{04}x(1 - 3y + 3y^2 - y^3 - 3x + 6xy - 3xy^2 + 3x^2 - 3x^2y - x^3) \\ &\quad - 5a_{05}x(1 - 4y + 6y^2 - 4y^3 + y^4 - 4x + 12xy - 12xy^2 + 4xy^3 + 6x^2 - 12x^2y + 6x^2y^2 - 4x^3 \\ &\quad + 4x^3y + x^4) - a_{11}xy - 2a_{12}xy(1 - x - y) - 3a_{13}xy(1 - 2y + y^2 - 2x + 2xy + x^2) \\ &\quad - 4a_{14}xy(1 - 3y + 3y^2 - y^3 - 3x + 6xy - 3xy^2 + 3x^2 - 3x^2y - x^3) - a_{21}xy^2 - 2a_{22}xy^2(1 - x - y) \\ &\quad - 3a_{23}xy^2(1 - 2y + y^2 - 2x + 2xy + x^2) - a_{31}xy^3 - 2a_{32}xy^3(1 - x - y) - a_{41}xy^4 = \\ &= -2a_{02}x + 2a_{02}x^2 + 2a_{02}xy - 3a_{03}x + 6a_{03}xy - 3a_{03}xy^2 + 6a_{03}x^2 - 6a_{03}x^2y - 3a_{03}x^3 - 4a_{04}x \\ &\quad + 12a_{04}xy - 12a_{04}xy^2 + 4a_{04}xy^3 + 12a_{04}x^2 - 24a_{04}x^2y + 12a_{04}x^2y^2 - 12a_{04}x^3 + 12a_{04}x^3y \\ &\quad + 4a_{04}x^4 - 5a_{05}x + 20a_{05}xy - 30a_{05}xy^2 + 20a_{05}xy^3 - 5a_{05}xy^4 + 20a_{05}x^2 - 60a_{05}x^2y \\ &\quad + 60a_{05}x^2y^2 - 20a_{05}x^2y^3 - 30a_{05}x^3 + 60a_{05}x^3y - 30a_{05}x^3y^2 + 20a_{05}x^4 - \mathbf{20a_{05}x^4y} - 5a_{05}x^5 \\ &\quad - a_{11}xy - 2a_{12}xy + 2a_{12}x^2y + 2a_{12}xy^2 - 3a_{13}xy + 6a_{13}xy^2 - 3a_{13}xy^3 + 6a_{13}x^2y - 6a_{13}x^2y^2 \\ &\quad - 3a_{13}x^3y - 4a_{14}xy + 12a_{14}xy^2 - 12a_{14}xy^3 + 4a_{14}xy^4 + 12a_{14}x^2y - 24a_{14}x^2y^2 + 12a_{14}x^2y^3 \\ &\quad - 12a_{14}x^3y + 12a_{14}x^3y^2 + \mathbf{4a_{14}x^4y} - a_{21}xy^2 - 2a_{22}xy^2 + 2a_{22}x^2y^2 + 2a_{22}xy^3 - 3a_{23}xy^2 \\ &\quad + 6a_{23}xy^3 - 3a_{23}xy^4 + 6a_{23}x^2y^2 - 6a_{23}x^2y^3 - 3a_{23}x^3y^2 - a_{31}xy^3 - 2a_{32}xy^3 + 2a_{32}x^2y^3 \\ &\quad + 2a_{32}xy^4 - a_{41}xy^4 = \\ &= x(-2a_{02} - 3a_{03} - 4a_{04} - 5a_{05}) + xy(2a_{02} + 6a_{03} + 12a_{04} + 20a_{05} - a_{11} - 2a_{12} - 3a_{13} - 4a_{14}) \\ &\quad + xy^2(-3a_{03} - 12a_{04} - 30a_{05} + 2a_{12} + 6a_{13} + 12a_{14} - a_{21} - 2a_{22} - 3a_{23}) \\ &\quad + xy^3(4a_{04} + 20a_{05} - 3a_{13} - 12a_{14} + 2a_{22} + 6a_{23} - a_{31} - 2a_{32}) \\ &\quad + xy^4(-5a_{05} + 4a_{14} - 3a_{23} + 2a_{32} - a_{41}) + x^2(2a_{02} + 6a_{03} + 12a_{04} + 20a_{05}) \\ &\quad + x^2y(-6a_{03} - 24a_{04} - 60a_{05} + 2a_{12} + 6a_{13} + 12a_{14}) \\ &\quad + x^2y^2(12a_{04} + 60a_{05} - 6a_{13} - 24a_{14} + 2a_{22} + 6a_{23}) + x^2y^3(-20a_{05} + 12a_{14} - 6a_{23} + 2a_{32}) \\ &\quad + x^3(-3a_{03} - 12a_{04} - 30a_{05}) + x^3y(12a_{04} + 60a_{05} - 3a_{13} - 12a_{14}) \\ &\quad + x^3y^2(-30a_{05} + 12a_{14} - 3a_{23}) + x^4(4a_{04} + 20a_{05}) + x^4y(-20a_{05} + 4a_{14}) + x^5(-5a_{05}) \end{aligned}$$

$$\begin{aligned}
& y \frac{\partial \varphi}{\partial x} = \\
& = 2b_{02}xy + 3b_{03}x^2y + 4b_{04}x^3y + 5b_{05}x^4y + b_{11}y(1-x-y) + 2b_{12}xy(1-x-y) \\
& + 3b_{13}x^2y(1-x-y) + 4b_{14}x^3y(1-x-y) + b_{21}y(1-2y+y^2-2x+2xy+x^2) \\
& + 2b_{22}xy(1-2y+y^2-2x+2xy+x^2) + 3b_{23}x^2y(1-2y+y^2-2x+2xy+x^2) \\
& + b_{31}y(1-3y+3y^2-y^3-3x+6xy-3xy^2+3x^2-3x^2y-x^3) \\
& + 2b_{32}xy(1-3y+3y^2-y^3-3x+6xy-3xy^2+3x^2-3x^2y-x^3) \\
& + b_{41}y(1-4y+6y^2-4y^3+y^4-4x+12xy-12xy^2+4xy^3+6x^2-12x^2y+6x^2y^2-4x^3 \\
& + 4x^3y+x^4) - b_{11}xy - b_{12}x^2y - b_{13}x^3y - b_{14}x^4y - 2b_{20}y(1-x-y) - 2b_{21}xy(1-x-y) \\
& - 2b_{22}x^2y(1-x-y) - 2b_{23}x^3y(1-x-y) - 3b_{30}y(1-2y+y^2-2x+2xy+x^2) \\
& - 3b_{31}xy(1-2y+y^2-2x+2xy+x^2) - 3b_{32}x^2y(1-2y+y^2-2x+2xy+x^2) \\
& - 4b_{40}y(1-3y+3y^2-y^3-3x+6xy-3xy^2+3x^2-3x^2y-x^3) \\
& - 4b_{41}xy(1-3y+3y^2-y^3-3x+6xy-3xy^2+3x^2-3x^2y-x^3) \\
& - 5b_{50}y(1-4y+6y^2-4y^3+y^4-4x+12xy-12xy^2+4xy^3+6x^2-12x^2y+6x^2y^2-4x^3 \\
& + 4x^3y+x^4) = \\
& = 2b_{02}xy + 3b_{03}x^2y + 4b_{04}x^3y + 5b_{05}x^4y + b_{11}y - b_{11}xy - b_{11}y^2 + 2b_{12}xy - 2b_{12}x^2y - 2b_{12}xy^2 \\
& + 3b_{13}x^2y - 3b_{13}x^3y - 3b_{13}x^2y^2 + 4b_{14}x^3y - 4b_{14}x^4y - 4b_{14}x^3y^2 + b_{21}y - 2b_{21}y^2 + b_{21}y^3 \\
& - 2b_{21}xy + 2b_{21}xy^2 + b_{21}x^2y + 2b_{22}xy - 4b_{22}xy^2 + 2b_{22}xy^3 - 4b_{22}x^2y + 4b_{22}x^2y^2 + 2b_{22}x^3y \\
& + 3b_{23}x^2y - 6b_{23}x^2y^2 + 3b_{23}x^2y^3 - 6b_{23}x^3y + 6b_{23}x^3y^2 + 3b_{23}x^4y + b_{31}y - 3b_{31}y^2 + 3b_{31}y^3 \\
& - b_{31}y^4 - 3b_{31}xy + 6b_{31}xy^2 - 3b_{31}xy^3 + 3b_{31}x^2y - 3b_{31}x^2y^2 - b_{31}x^3y + 2b_{32}xy - 6b_{32}xy^2 \\
& + 6b_{32}xy^3 - 2b_{32}xy^4 - 6b_{32}x^2y + 12b_{32}x^2y^2 - 6b_{32}x^2y^3 + 6b_{32}x^3y - 6b_{32}x^3y^2 - 2b_{32}x^4y + b_{41}y \\
& - 4b_{41}y^2 + 6b_{41}y^3 - 4b_{41}y^4 + b_{41}y^5 - 4b_{41}xy + 12b_{41}xy^2 - 12b_{41}xy^3 + 4b_{41}xy^4 + 6b_{41}x^2y \\
& - 12b_{41}x^2y^2 + 6b_{41}x^2y^3 - 4b_{41}x^3y + 4b_{41}x^3y^2 + b_{41}x^4y - b_{11}xy - b_{12}x^2y - b_{13}x^3y - b_{14}x^4y \\
& - 2b_{20}y + 2b_{20}xy + 2b_{20}y^2 - 2b_{21}xy + 2b_{21}x^2y + 2b_{21}xy^2 - 2b_{22}x^2y + 2b_{22}x^3y + 2b_{22}x^2y^2 \\
& - 2b_{23}x^3y + 2b_{23}x^4y + 2b_{23}x^3y^2 - 3b_{30}y + 6b_{30}y^2 - 3b_{30}y^3 + 6b_{30}xy - 6b_{30}xy^2 - 3b_{30}x^2y \\
& - 3b_{31}xy + 6b_{31}xy^2 - 3b_{31}xy^3 + 6b_{31}x^2y - 6b_{31}x^2y^2 - 3b_{31}x^3y - 3b_{32}x^2y + 6b_{32}x^2y^2 - 3b_{32}x^2y^3 \\
& + 6b_{32}x^3y - 6b_{32}x^3y^2 - 3b_{32}x^4y - 4b_{40}y + 12b_{40}y^2 - 12b_{40}y^3 + 4b_{40}y^4 + 12b_{40}xy - 24b_{40}xy^2 \\
& + 12b_{40}xy^3 - 12b_{40}x^2y + 12b_{40}x^2y^2 + 4b_{40}x^3y - 4b_{41}xy + 12b_{41}xy^2 - 12b_{41}xy^3 + 4b_{41}xy^4 \\
& + 12b_{41}x^2y - 24b_{41}x^2y^2 + 12b_{41}x^2y^3 - 12b_{41}x^3y + 12b_{41}x^3y^2 + 4b_{41}x^4y - 5b_{50}y + 20b_{50}y^2 \\
& - 30b_{50}y^3 + 20b_{50}y^4 - 5b_{50}y^5 + 20b_{50}xy - 60b_{50}xy^2 + 60b_{50}xy^3 - 20b_{50}xy^4 - 30b_{50}x^2y \\
& + 60b_{50}x^2y^2 - 30b_{50}x^2y^3 + 20b_{50}x^3y - 20b_{50}x^3y^2 - 5b_{50}x^4y = \\
& = y(b_{11} + b_{21} + b_{31} + b_{41} - 2b_{20} - 3b_{30} - 4b_{40} - 5b_{50}) \\
& + y^2(-b_{11} - 2b_{21} - 3b_{31} - 4b_{41} + 2b_{20} + 6b_{30} + 12b_{40} + 20b_{50}) \\
& + y^3(b_{21} + 3b_{31} + 6b_{41} - 3b_{30} - 12b_{40} - 30b_{50}) + y^4(-3b_{31} - 4b_{41} + 4b_{40} + 20b_{50}) \\
& + y^5(b_{41} - 5b_{50}) \\
& + xy(2b_{02} - 2b_{11} + 2b_{12} - 4b_{21} + 2b_{22} - 6b_{31} + 2b_{32} - 8b_{41} + 6b_{30} + 12b_{40} + 20b_{50}) \\
& + xy^2(-2b_{12} + 4b_{21} - 4b_{22} + 12b_{31} - 6b_{32} + 24b_{41} - 6b_{30} - 24b_{40} - 60b_{50}) \\
& + xy^3(2b_{22} - 6b_{31} + 6b_{32} - 24b_{41} + 12b_{40} + 60b_{50}) + xy^4(-2b_{32} + 8b_{41} - 20b_{50}) \\
& + x^2y(3b_{03} - 3b_{12} + 3b_{13} + 3b_{21} - 6b_{22} + 3b_{23} + 9b_{31} - 9b_{32} + 18b_{41} - 3b_{30} - 12b_{40} - 30b_{50}) \\
& + x^2y^2(-3b_{13} + 6b_{22} - 6b_{23} - 9b_{31} + 18b_{32} - 36b_{41} + 12b_{40} + 60b_{50}) \\
& + x^2y^3(3b_{23} - 9b_{32} + 18b_{41} - 30b_{50}) \\
& + x^3y(4b_{04} - 4b_{13} + 4b_{14} + 4b_{22} - 8b_{23} - 4b_{31} + 12b_{32} - 16b_{41} + 4b_{40} + 20b_{50}) \\
& + x^3y^2(-4b_{14} + 8b_{23} - 12b_{32} + 16b_{41} - 20b_{50}) + x^4y(5b_{05} - 5b_{14} + 5b_{23} - 5b_{32} + 5b_{41} - 5b_{50})
\end{aligned}$$

$$\begin{aligned}
& z \frac{\partial \xi}{\partial x} = \\
& = c_{11}y(1-x-y) + c_{12}y^2(1-x-y) + c_{13}y^3(1-x-y) + c_{14}y^4(1-x-y) + 2c_{20}x(1-x-y) \\
& + 2c_{21}xy(1-x-y) + 2c_{22}xy^2(1-x-y) + 2c_{23}xy^3(1-x-y) + 3c_{30}x^2(1-x-y) \\
& + 3c_{31}x^2y(1-x-y) + 3c_{32}x^2y^2(1-x-y) + 4c_{40}x^3(1-x-y) + 4c_{41}x^3y(1-x-y) \\
& + 5c_{50}x^4(1-x-y) =
\end{aligned}$$

$$\begin{aligned}
&= c_{11}y - c_{11}xy - c_{11}y^2 + c_{12}y^2 - c_{12}xy^2 - c_{12}y^3 + c_{13}y^3 - c_{13}xy^3 - c_{13}y^4 + c_{14}y^4 - c_{14}xy^4 - c_{14}y^5 \\
&+ 2c_{20}x - 2c_{20}x^2 - 2c_{20}xy + 2c_{21}xy - 2c_{21}x^2y - 2c_{21}xy^2 + 2c_{22}xy^2 - 2c_{22}x^2y^2 - 2c_{22}xy^3 \\
&+ 2c_{23}xy^3 - 2c_{23}x^2y^3 - 2c_{23}xy^4 + 3c_{30}x^2 - 3c_{30}x^3 - 3c_{30}x^2y + 3c_{31}x^2y - 3c_{31}x^3y - 3c_{31}x^2y^2 \\
&+ 3c_{32}x^2y^2 - 3c_{32}x^3y^2 - 3c_{32}x^2y^3 + 4c_{40}x^3 - 4c_{40}x^4 - 4c_{40}x^3y + 4c_{41}x^3y - 4c_{41}x^4y - 4c_{41}x^3y^2 \\
&+ 5c_{50}x^4 - 5c_{50}x^5 - 5c_{50}x^4y = \\
&= y(c_{11}) + y^2(-c_{11} + c_{12}) + y^3(-c_{12} + c_{13}) + y^4(-c_{13} + c_{14}) + y^5(-c_{14}) + x(2c_{20}) \\
&+ xy(-c_{11} - 2c_{20} + 2c_{21}) + xy^2(-c_{12} - 2c_{21} + 2c_{22}) + xy^3(-c_{13} - 2c_{22} + 2c_{23}) + xy^4(-c_{14} - 2c_{23}) \\
&+ x^2(-2c_{20} + 3c_{30}) + x^2y(-2c_{21} - 3c_{30} + 3c_{31}) + x^2y^2(-2c_{22} - 3c_{31} + 3c_{32}) + x^2y^3(-2c_{23} - 3c_{32}) \\
&+ x^3(-3c_{30} + 4c_{40}) + x^3y(-3c_{31} - 4c_{40} + 4c_{41}) + x^3y^2(-3c_{32} - 4c_{41}) + x^4(-4c_{40} + 5c_{50}) \\
&+ x^4y(-4c_{41} - 5c_{50}) + x^5(-5c_{50})
\end{aligned}$$

$$\begin{aligned}
&x \frac{\partial f}{\partial x} + y \frac{\partial \varphi}{\partial x} + z \frac{\partial \xi}{\partial x} = \\
&= y(b_{11} + b_{21} + b_{31} + b_{41} - 2b_{20} - 3b_{30} - 4b_{40} - 5b_{50} + c_{11}) \\
&+ y^2(-b_{11} - 2b_{21} - 3b_{31} - 4b_{41} + 2b_{20} + 6b_{30} + 12b_{40} + 20b_{50} - c_{11} + c_{12}) \\
&+ y^3(b_{21} + 3b_{31} + 6b_{41} - 3b_{30} - 12b_{40} - 30b_{50} - c_{12} + c_{13}) \\
&+ y^4(-3b_{31} - 4b_{41} + 4b_{40} + 20b_{50} - c_{13} + c_{14}) + y^5(b_{41} - 5b_{50} - c_{14}) \\
&+ x(-2a_{02} - 3a_{03} - 4a_{04} - 5a_{05} + 2c_{20}) \\
&+ xy(2a_{02} + 6a_{03} + 12a_{04} + 20a_{05} - a_{11} - 2a_{12} - 3a_{13} - 4a_{14} + 2b_{02} - 2b_{11} + 2b_{12} - 4b_{21} + 2b_{22} \\
&- 6b_{31} + 2b_{32} - 8b_{41} + 6b_{30} + 12b_{40} + 20b_{50} - c_{11} - 2c_{20} + 2c_{21}) \\
&+ xy^2(-3a_{03} - 12a_{04} - 30a_{05} + 2a_{12} + 6a_{13} + 12a_{14} - a_{21} - 2a_{22} - 3a_{23} - 2b_{12} + 4b_{21} - 4b_{22} \\
&+ 12b_{31} - 6b_{32} + 24b_{41} - 6b_{30} - 24b_{40} - 60b_{50} - c_{12} - 2c_{21} + 2c_{22}) \\
&+ xy^3(4a_{04} + 20a_{05} - 3a_{13} - 12a_{14} + 2a_{22} + 6a_{23} - a_{31} - 2a_{32} + 2b_{22} - 6b_{31} + 6b_{32} - 24b_{41} \\
&+ 12b_{40} + 60b_{50} - c_{13} - 2c_{22} + 2c_{23}) \\
&+ xy^4(-5a_{05} + 4a_{14} - 3a_{23} + 2a_{32} - a_{41} - 2b_{32} + 8b_{41} - 20b_{50} - c_{14} - 2c_{23}) \\
&+ x^2(2a_{02} + 6a_{03} + 12a_{04} + 20a_{05} - 2c_{20} + 3c_{30}) \\
&+ x^2y(-6a_{03} - 24a_{04} - 60a_{05} + 2a_{12} + 6a_{13} + 12a_{14} + 3b_{03} - 3b_{12} + 3b_{13} + 3b_{21} - 6b_{22} + 3b_{23} \\
&+ 9b_{31} - 9b_{32} + 18b_{41} - 3b_{30} - 12b_{40} - 30b_{50} - 2c_{21} - 3c_{30} + 3c_{31}) \\
&+ x^2y^2(12a_{04} + 60a_{05} - 6a_{13} - 24a_{14} + 2a_{22} + 6a_{23} - 3b_{13} + 6b_{22} - 6b_{23} - 9b_{31} + 18b_{32} - 36b_{41} \\
&+ 12b_{40} + 60b_{50} - 2c_{22} - 3c_{31} + 3c_{32}) \\
&+ x^2y^3(-20a_{05} + 12a_{14} - 6a_{23} + 2a_{32} + 3b_{23} - 9b_{32} + 18b_{41} - 30b_{50} - 2c_{23} - 3c_{32}) \\
&+ x^3(-3a_{03} - 12a_{04} - 30a_{05} - 3c_{30} + 4c_{40}) \\
&+ x^3y(12a_{04} + 60a_{05} - 3a_{13} - 12a_{14} + 4b_{04} - 4b_{13} + 4b_{14} + 4b_{22} - 8b_{23} - 4b_{31} + 12b_{32} - 16b_{41} \\
&+ 4b_{40} + 20b_{50} - 3c_{31} - 4c_{40} + 4c_{41}) \\
&+ x^3y^2(-30a_{05} + 12a_{14} - 3a_{23} - 4b_{14} + 8b_{23} - 12b_{32} + 16b_{41} - 20b_{50} - 3c_{32} - 4c_{41}) \\
&+ x^4(4a_{04} + 20a_{05} - 4c_{40} + 5c_{50}) \\
&+ x^4y(-20a_{05} + 4a_{14} + 5b_{05} - 5b_{14} + 5b_{23} - 5b_{32} + 5b_{41} - 5b_{50} - 4c_{41} - 5c_{50}) + x^5(-5a_{05} - 5c_{50})
\end{aligned}$$

Coefficients that are expressed through the parameters  $A_i$ ,  $B_i$ ,  $\alpha_i$  and  $\beta_i$  in accordance with formulas (5–7), are marked in blue, and those in red are those that give in sum zero.

Similarly, for the second equality from system (8):

$$x \frac{\partial f[y; z(x, y)]}{\partial y} = x \frac{\partial f}{\partial y} + x \frac{\partial f}{\partial z} \frac{\partial z}{\partial y} = x \frac{\partial f}{\partial y} - x \frac{\partial f}{\partial z} =$$

$$\begin{aligned}
&= (a_{11} - 2a_{02})(x - x^2 - xy) + (a_{12} - 3a_{03})(x - 2xy + xy^2 - 2x^2 + 2x^2y + x^3) \\
&+ (a_{13} - 4a_{04})(x - 3xy + 3xy^2 - xy^3 - 3x^2 + 6x^2y - 3x^2y^2 + 3x^3 - 3x^3y - x^4) \\
&+ (a_{14} - 5a_{05})(x - 4xy + 6xy^2 - 4xy^3 + xy^4 - 4x^2 + 12x^2y - 12x^2y^2 + 4x^2y^3 + 6x^3 - 12x^3y \\
&+ 6x^3y^2 - 4x^4 + 4x^4y + x^5) + (2a_{20} - a_{11})xy + (2a_{21} - 2a_{12})(xy - x^2y - xy^2) \\
&+ (2a_{22} - 3a_{13})(xy - 2xy^2 + xy^3 - 2x^2y + 2x^2y^2 + x^3y) \\
&+ (2a_{23} - 4a_{14})(xy - 3xy^2 + 3xy^3 - xy^4 - 3x^2y + 6x^2y^2 - 3x^2y^3 + 3x^3y - 3x^3y^2 - x^4y) \\
&+ (3a_{30} - a_{21})xy^2 + (3a_{31} - 2a_{22})(xy^2 - x^2y^2 - xy^3) \\
&+ (3a_{32} - 3a_{23})(xy^2 - 2xy^3 + xy^4 - 2x^2y^2 + 2x^2y^3 + x^3y^2) + (4a_{40} - a_{31})xy^3 \\
&+ (4a_{41} - 2a_{32})(xy^3 - x^2y^3 - xy^4) + (5a_{50} - a_{41})xy^4 = \\
&= x(a_{11} - 2a_{02} + a_{12} - 3a_{03} + a_{13} - 4a_{04} + a_{14} - 5a_{05}) \\
&+ xy(-2a_{11} + 2a_{02} - 4a_{12} + 6a_{03} - 6a_{13} + 12a_{04} - 8a_{14} + 20a_{05} + 2a_{20} + 2a_{21} + 2a_{22} + 2a_{23}) \\
&+ xy^2(3a_{12} - 3a_{03} + 9a_{13} - 12a_{04} + 18a_{14} - 30a_{05} - 3a_{21} - 6a_{22} - 9a_{23} + 3a_{30} + 3a_{31} + 3a_{32}) \\
&+ xy^3(-4a_{13} + 4a_{04} - 16a_{14} + 20a_{05} + 4a_{22} + 12a_{23} - 4a_{31} - 8a_{32} + 4a_{40} + 4a_{41}) \\
&+ xy^4(5a_{14} - 5a_{05} - 5a_{23} + 5a_{32} - 5a_{41} + 5a_{50}) \\
&+ x^2(-a_{11} + 2a_{02} - 2a_{12} + 6a_{03} - 3a_{13} + 12a_{04} - 4a_{14} + 20a_{05}) \\
&+ x^2y(4a_{12} - 6a_{03} + 12a_{13} - 24a_{04} + 24a_{14} - 60a_{05} - 2a_{21} - 4a_{22} - 6a_{23}) \\
&+ x^2y^2(-9a_{13} + 12a_{04} - 36a_{14} + 60a_{05} + 6a_{22} + 18a_{23} - 3a_{31} - 6a_{32}) \\
&+ x^2y^3(16a_{14} - 20a_{05} - 12a_{23} + 8a_{32} - 4a_{41}) + x^3(a_{12} - 3a_{03} + 3a_{13} - 12a_{04} + 6a_{14} - 30a_{05}) \\
&+ x^3y(-6a_{13} + 12a_{04} - 24a_{14} + 60a_{05} + 2a_{22} + 6a_{23}) + x^3y^2(18a_{14} - 30a_{05} - 9a_{23} + 3a_{32}) \\
&+ x^4(-a_{13} + 4a_{04} - 4a_{14} + 20a_{05}) + x^4y(8a_{14} - 20a_{05} - 2a_{23}) + x^5(a_{14} - 5a_{05})
\end{aligned}$$

$$\begin{aligned}
&y \frac{\partial \varphi[z(x, y), x]}{\partial y} = y \frac{\partial \varphi}{\partial z} \cdot \frac{\partial z}{\partial y} = -y \frac{\partial \varphi}{\partial z} = \\
&= -b_{11}xy - b_{12}x^2y - b_{13}x^3y - b_{14}x^4y - 2b_{20}y(1 - x - y) - 2b_{21}xy(1 - x - y) \\
&- 2b_{22}x^2y(1 - x - y) - 2b_{23}x^3y(1 - x - y) - 3b_{30}y(1 - 2y + y^2 - 2x + 2xy + x^2) \\
&- 3b_{31}xy(1 - 2y + y^2 - 2x + 2xy + x^2) - 3b_{32}x^2y(1 - 2y + y^2 - 2x + 2xy + x^2) \\
&- 4b_{40}y(1 - 3y + 3y^2 - y^3 - 3x + 6xy - 3xy^2 + 3x^2 - 3x^2y - x^3) \\
&- 4b_{41}xy(1 - 3y + 3y^2 - y^3 - 3x + 6xy - 3xy^2 + 3x^2 - 3x^2y - x^3) \\
&- 5b_{50}y(1 - 4y + 6y^2 - 4y^3 + y^4 - 4x + 12xy - 12xy^2 + 4xy^3 + 6x^2 - 12x^2y + 6x^2y^2 - 4x^3 \\
&+ 4x^3y + x^4) = \\
&= -b_{11}xy - b_{12}x^2y - b_{13}x^3y - b_{14}x^4y - 2b_{20}(y - xy - y^2) - 2b_{21}(xy - x^2y - xy^2) \\
&- 2b_{22}(x^2y - x^3y - x^2y^2) - 2b_{23}(x^3y - x^4y - x^3y^2) - 3b_{30}(y - 2y^2 + y^3 - 2xy + 2xy^2 + x^2y) \\
&- 3b_{31}(xy - 2xy^2 + xy^3 - 2x^2y + 2x^2y^2 + x^3y) \\
&- 3b_{32}(x^2y - 2x^2y^2 + x^2y^3 - 2x^3y + 2x^3y^2 + x^4y) \\
&- 4b_{40}(y - 3y^2 + 3y^3 - y^4 - 3xy + 6xy^2 - 3xy^3 + 3x^2y - 3x^2y^2 - x^3y) \\
&- 4b_{41}(xy - 3xy^2 + 3xy^3 - xy^4 - 3x^2y + 6x^2y^2 - 3x^2y^3 + 3x^3y - 3x^3y^2 - x^4y) \\
&- 5b_{50}(y - 4y^2 + 6y^3 - 4y^4 + y^5 - 4xy + 12xy^2 - 12xy^3 + 4xy^4 + 6x^2y - 12x^2y^2 + 6x^2y^3 - 4x^3y \\
&+ 4x^3y^2 + x^4y) = \\
&= y(-2b_{20} - 3b_{30} - 4b_{40} - 5b_{50}) + y^2(2b_{20} + 6b_{30} + 12b_{40} + 20b_{50}) + y^3(-3b_{30} - 12b_{40} - 30b_{50}) \\
&+ y^4(4b_{40} + 20b_{50}) + y^5(-5b_{50}) + xy(-b_{11} + 2b_{20} - 2b_{21} + 6b_{30} - 3b_{31} + 12b_{40} - 4b_{41} + 20b_{50}) \\
&+ xy^2(2b_{21} - 6b_{30} + 6b_{31} - 24b_{40} + 12b_{41} - 60b_{50}) + xy^3(-3b_{31} + 12b_{40} - 12b_{41} + 60b_{50}) \\
&+ xy^4(4b_{41} - 20b_{50}) + x^2y(-b_{12} + 2b_{21} - 2b_{22} - 3b_{30} + 6b_{31} - 3b_{32} - 12b_{40} + 12b_{41} - 30b_{50}) \\
&+ x^2y^2(2b_{22} - 6b_{31} + 6b_{32} + 12b_{40} - 24b_{41} + 60b_{50}) + x^2y^3(-3b_{32} + 12b_{41} - 30b_{50}) \\
&+ x^3y(-b_{13} + 2b_{22} - 2b_{23} - 3b_{31} + 6b_{32} + 4b_{40} - 12b_{41} + 20b_{50}) \\
&+ x^3y^2(2b_{23} - 3b_{32} + 12b_{41} - 20b_{50}) + x^4y(-b_{14} + 2b_{23} - 3b_{32} + 4b_{41} - 5b_{50})
\end{aligned}$$



$$\begin{aligned}
z \frac{\partial \xi}{\partial y} &= \\
&= 2c_{02}(y - xy - y^2) + 3c_{03}(y^2 - xy^2 - y^3) + 4c_{04}(y^3 - xy^3 - y^4) + 5c_{05}(y^4 - xy^4 - y^5) \\
&+ c_{11}(x - x^2 - xy) + 2c_{12}(xy - x^2y - xy^2) + 3c_{13}(xy^2 - x^2y^2 - xy^3) + 4c_{14}(xy^3 - x^2y^3 - xy^4) \\
&+ c_{21}(x^2 - x^3 - x^2y) + 2c_{22}(x^2y - x^3y - x^2y^2) + 3c_{23}(x^2y^2 - x^3y^2 - x^2y^3) + c_{31}(x^3 - x^4 - x^3y) \\
&+ 2c_{32}(x^3y - x^4y - x^3y^2) + c_{41}(x^4 - x^5 - x^4y) = \\
&= y(2c_{02}) + y^2(-2c_{02} + 3c_{03}) + y^3(-3c_{03} + 4c_{04}) + y^4(-4c_{04} + 5c_{05}) + y^5(-5c_{05}) + x(c_{11}) \\
&+ xy(-2c_{02} - c_{11} + 2c_{12}) + xy^2(-3c_{03} - 2c_{12} + 3c_{13}) + xy^3(-4c_{04} - 3c_{13} + 4c_{14}) \\
&+ xy^4(-5c_{05} - 4c_{14}) + x^2(-c_{11} + c_{21}) + x^2y(-2c_{12} - c_{21} + 2c_{22}) + x^2y^2(-3c_{13} - 2c_{22} + 3c_{23}) \\
&+ x^2y^3(-4c_{14} - 3c_{23}) + x^3(-c_{21} + c_{31}) + x^3y(-2c_{22} - c_{31} + 2c_{32}) + x^3y^2(-3c_{23} - 2c_{32}) \\
&+ x^4(-c_{31} + c_{41}) + x^4y(-2c_{32} - c_{41}) + x^5(-c_{41})
\end{aligned}$$

$$\begin{aligned}
x \frac{\partial f}{\partial y} + y \frac{\partial \varphi}{\partial y} + z \frac{\partial \xi}{\partial y} &= \\
&= y(-2b_{20} - 3b_{30} - 4b_{40} - 5b_{50} + 2c_{02}) + y^2(2b_{20} + 6b_{30} + 12b_{40} + 20b_{50} - 2c_{02} + 3c_{03}) \\
&+ y^3(-3b_{30} - 12b_{40} - 30b_{50} - 3c_{03} + 4c_{04}) + y^4(4b_{40} + 20b_{50} - 4c_{04} + 5c_{05}) + y^5(-5b_{50} - 5c_{05}) \\
&+ x(a_{11} - 2a_{02} + a_{12} - 3a_{03} + a_{13} - 4a_{04} + a_{14} - 5a_{05} + c_{11}) \\
&+ xy(-2a_{11} + 2a_{02} - 4a_{12} + 6a_{03} - 6a_{13} + 12a_{04} - 8a_{14} + 20a_{05} + 2a_{20} + 2a_{21} + 2a_{22} + 2a_{23} - b_{11} \\
&+ 2b_{20} - 2b_{21} + 6b_{30} - 3b_{31} + 12b_{40} - 4b_{41} + 20b_{50} - 2c_{02} - c_{11} + 2c_{12}) \\
&+ xy^2(3a_{12} - 3a_{03} + 9a_{13} - 12a_{04} + 18a_{14} - 30a_{05} - 3a_{21} - 6a_{22} - 9a_{23} + 3a_{30} + 3a_{31} + 3a_{32} \\
&+ 2b_{21} - 6b_{30} + 6b_{31} - 24b_{40} + 12b_{41} - 60b_{50} - 3c_{03} - 2c_{12} + 3c_{13}) \\
&+ xy^3(-4a_{13} + 4a_{04} - 16a_{14} + 20a_{05} + 4a_{22} + 12a_{23} - 4a_{31} - 8a_{32} + 4a_{40} + 4a_{41} - 3b_{31} + 12b_{40} \\
&- 12b_{41} + 60b_{50} - 4c_{04} - 3c_{13} + 4c_{14}) \\
&+ xy^4(5a_{14} - 5a_{05} - 5a_{23} + 5a_{32} - 5a_{41} + 5a_{50} + 4b_{41} - 20b_{50}) \\
&+ x^2(-a_{11} + 2a_{02} - 2a_{12} + 6a_{03} - 3a_{13} + 12a_{04} - 4a_{14} + 20a_{05} - c_{11} + c_{21}) \\
&+ x^2y(4a_{12} - 6a_{03} + 12a_{13} - 24a_{04} + 24a_{14} - 60a_{05} - 2a_{21} - 4a_{22} - 6a_{23} - b_{12} + 2b_{21} - 2b_{22} \\
&- 3b_{30} + 6b_{31} - 3b_{32} - 12b_{40} + 12b_{41} - 30b_{50} - 2c_{12} - c_{21} + 2c_{22}) \\
&+ x^2y^2(-9a_{13} + 12a_{04} - 36a_{14} + 60a_{05} + 6a_{22} + 18a_{23} - 3a_{31} - 6a_{32} + 2b_{22} - 6b_{31} + 6b_{32} + 12b_{40} \\
&- 24b_{41} + 60b_{50} - 3c_{13} - 2c_{22} + 3c_{23}) \\
&+ x^2y^3(16a_{14} - 20a_{05} - 12a_{23} + 8a_{32} - 4a_{41} - 3b_{32} + 12b_{41} - 30b_{50} - 4c_{14} - 3c_{23}) \\
&+ x^3(a_{12} - 3a_{03} + 3a_{13} - 12a_{04} + 6a_{14} - 30a_{05} - c_{21} + c_{31}) \\
&+ x^3y(-6a_{13} + 12a_{04} - 24a_{14} + 60a_{05} + 2a_{22} + 6a_{23} - b_{13} + 2b_{22} - 2b_{23} - 3b_{31} + 6b_{32} + 4b_{40} \\
&- 12b_{41} + 20b_{50} - 2c_{22} - c_{31} + 2c_{32}) \\
&+ x^3y^2(18a_{14} - 30a_{05} - 9a_{23} + 3a_{32} + 2b_{23} - 3b_{32} + 12b_{41} - 20b_{50} - 3c_{23} - 2c_{32}) \\
&+ x^4(-a_{13} + 4a_{04} - 4a_{14} + 20a_{05} - c_{31} + c_{41}) \\
&+ x^4y(8a_{14} - 20a_{05} - 2a_{23} - b_{14} + 2b_{23} - 3b_{32} + 4b_{41} - 5b_{50} - 2c_{32} - c_{41}) + x^5(a_{14} - 5a_{05} - c_{41})
\end{aligned}$$

Equating the coefficients at the same powers of  $x$ ,  $y$  and  $z$  to zero, we obtain a system of 30 linear equations with 30 unknown parameters.