$k_{10} := 8.936 \cdot 10^5 \cdot \frac{mol}{s \cdot m^3 \cdot bar^2}$ $E_1 := 63266 \cdot \frac{J}{mol}$ $k_{20} := 50.752 \cdot \frac{mol}{s \cdot m^3 \cdot bar^2}$ $E_2 := 15956 \cdot \frac{J}{mol}$ $R_g := 8.314 \cdot \frac{J}{mol \cdot K}$

$P := 2 \cdot bar$ $n_{A0} := 2.144 \cdot 10^{-2} \cdot \frac{mol}{s}$ $n_{B0} := 3 \cdot n_{A0}$ $D := 50.8 \cdot mm$ $T_0 := 200\,°C$ $T_w := T_0$ $T_{rif} := T_0$ $U := 28.38 \cdot \frac{W}{m^2 \cdot K}$

$C_{PA} := 36.0 \cdot \frac{J}{mol \cdot K}$ $C_{PB} := 105.9 \cdot \frac{J}{mol \cdot K}$ $C_{PC} := 30.1 \cdot \frac{J}{mol \cdot K}$ $C_{PD} := 117.2 \cdot \frac{J}{mol \cdot K}$ $C_{PE} := 128.5 \cdot \frac{J}{mol \cdot K}$

$n_0 := n_{A0} + n_{B0} = 0.086 \frac{mol}{s}$ $y_A(X_1, X_2) := \frac{n_{A0} - n_{A0} \cdot (X_1 + X_2)}{n_0 - n_{A0} \cdot X_2}$ $y_B(X_1, X_2) := \frac{n_{B0} - n_{A0} \cdot (X_1 + X_2)}{n_0 - n_{A0} \cdot X_2}$

$k_1(T) := k_{10} \cdot \exp\left(-\frac{E_1}{R_g \cdot T}\right)$ $r_1(T, X_1, X_2) := -k_1(T) \cdot P^2 \cdot y_A(X_1, X_2) \cdot y_B(X_1, X_2)$ $\Delta H_1 := -111790 \cdot \frac{J}{mol}$

$k_2(T) := k_{20} \cdot \exp\left(-\frac{E_2}{R_g \cdot T}\right)$ $r_2(T, X_1, X_2) := -k_2(T) \cdot P^2 \cdot y_A(X_1, X_2) \cdot y_B(X_1, X_2)$ $\Delta H_2 := -184220 \cdot \frac{J}{mol}$

$\Sigma nC_P(X_1, X_2) := n_{A0} \cdot (1 - X_1 - X_2) \cdot C_{PA} + \left[n_{B0} - n_{A0} \cdot (X_1 + X_2)\right] \cdot C_{PB} \cdots$
$+ n_{A0} \cdot X_1 \cdot C_{PC} + n_{A0} \cdot X_1 \cdot C_{PD} + n_{A0} \cdot X_2 \cdot C_{PE}$

$T_m(\alpha, X_1, X_2) := T_{rif} + \frac{\alpha}{\Sigma nC_P(X_1, X_2)}$

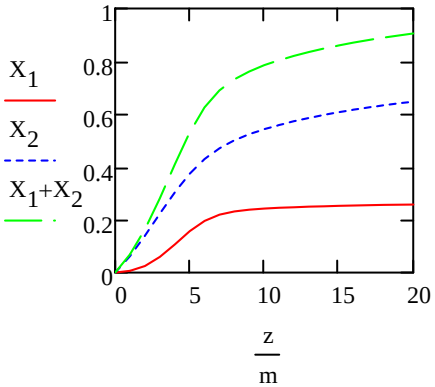
$dX_1(T, X_1, X_2) := \frac{\pi \cdot D^2}{4} \cdot \frac{-r_1(T, X_1, X_2)}{n_{A0}}$ $dX_2(T, X_1, X_2) := \frac{\pi \cdot D^2}{4} \cdot \frac{-r_2(T, X_1, X_2)}{n_{A0}}$

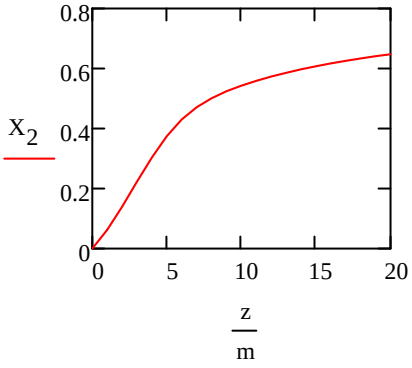
$d\alpha(T, X_1, X_2) := \left[\left(-r_1(T, X_1, X_2)\right) \cdot (-\Delta H_1) + \left(-r_2(T, X_1, X_2)\right) \cdot (-\Delta H_2) + U \cdot (T_w - T) \cdot \frac{4}{D}\right] \cdot \frac{\pi \cdot D^2}{4}$

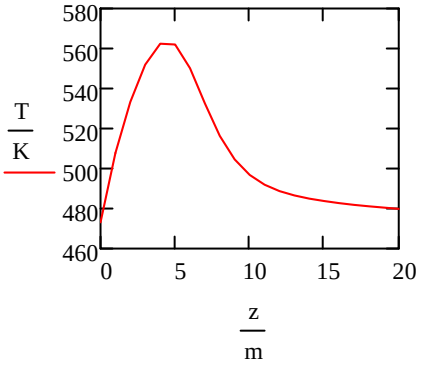
$\Delta z := 1 \cdot m$ $\begin{pmatrix} X1_0 \\ X2_0 \\ \alpha_0 \end{pmatrix} := \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$ $z_0 := 0 \cdot cm$ $N := 20$ $i := 1 .. N$ $z_i := i \cdot \Delta z$

$$\begin{pmatrix} X1_i \\ X2_i \\ \alpha_i \end{pmatrix} := \begin{pmatrix} X1_{i-1} \\ X2_{i-1} \\ \alpha_{i-1} \end{pmatrix} + \Delta z \cdot \begin{bmatrix} dX1\left[T_m\left[\alpha_{i-1} \cdot (W), X1_{i-1}, X2_{i-1}\right], X1_{i-1}, X2_{i-1}\right] \\ dX2\left[T_m\left[\alpha_{i-1} \cdot (W), X1_{i-1}, X2_{i-1}\right], X1_{i-1}, X2_{i-1}\right] \\ d\alpha\left[T_m\left[\alpha_{i-1} \cdot (W), X1_{i-1}, X2_{i-1}\right], X1_{i-1}, X2_{i-1}\right] \cdot \left(\frac{1}{W}\right) \end{bmatrix}$$

$i := 0 .. N$ $\alpha := \alpha \cdot W$ $T_i := T_m(\alpha_i, X1_i, X2_i)$







z_i =		$X1_i$ =	$X2_i$ =	α_i =		T_i =		$-r1\left(T_i, X1_i, X2_i\right)$ =		$-r2\left(T_i, X1_i, X2_i\right)$ =	
0	·m	0.0000	0.0000	0	W	473.15	·K	0.0694	$\cdot\frac{mol}{m^3 \cdot s}$	0.6591	$\cdot\frac{mol}{m^3 \cdot s}$
1		0.0066	0.0623	261.825		507.755		0.1950		0.8158	
2		0.0250	0.1394	453.873		533.296		0.3611		0.8830	
3		0.0591	0.2229	592.95		551.935		0.5030		0.8579	
4		0.1067	0.3040	670.405		562.438		0.5314		0.7476	
5		0.1569	0.3747	665.543		561.962		0.4137		0.5871	
6		0.1960	0.4302	576.236		550.162		0.2449		0.4318	
7		0.2192	0.4710	444.162		532.582		0.1280		0.3176	
8		0.2313	0.5010	322.581		516.356		0.0705		0.2447	
9		0.2380	0.5242	234.244		504.549		0.0444		0.1994	
10		0.2422	0.5430	176.53		496.828		0.0317		0.1698	
11		0.2452	0.5591	139.879		491.923		0.0248		0.1490	
12		0.2475	0.5731	116.115		488.741		0.0206		0.1332	
13		0.2495	0.5857	99.884		486.568		0.0177		0.1203	
14		0.2511	0.5971	88.039		484.982		0.0155		0.1095	
15		0.2526	0.6074	78.82		483.747		0.0137		0.1000	
16		0.2539	0.6169	71.261		482.734		0.0122		0.0916	
17		0.2550	0.6256	64.826		481.871		0.0110		0.0841	
18		0.2561	0.6335	59.211		481.118		0.0099		0.0773	
19		0.2570	0.6408	54.234		480.45		0.0090		0.0712	
20		0.2579	0.6475	49.778		479.852		0.0082		0.0656	

$$d\alpha(T, X_1, X_2) := \left[\left(-r_1(T, X_1, X_2)\right)\cdot\left(-\Delta H_1\right) + \left(-r_2(T, X_1, X_2)\right)\cdot\left(-\Delta H_2\right) + 0\cdot U\cdot\left(T_w - T\right)\cdot\frac{4}{D} \right]\cdot\frac{\pi\cdot D^2}{4} \qquad \alpha := 0$$

$\Delta z_a := 1\cdot mm$

$$\begin{pmatrix} X1a_0 \\ X2a_0 \\ \alpha a_0 \end{pmatrix} := \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

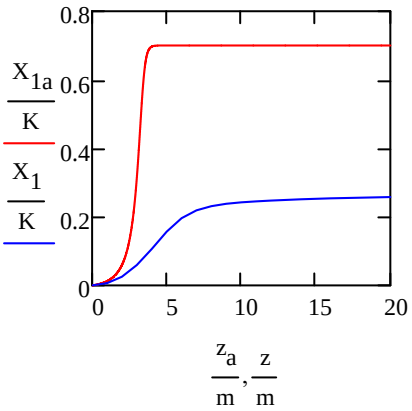
$z_{a_0} := 0\cdot cm \qquad N := 20000$

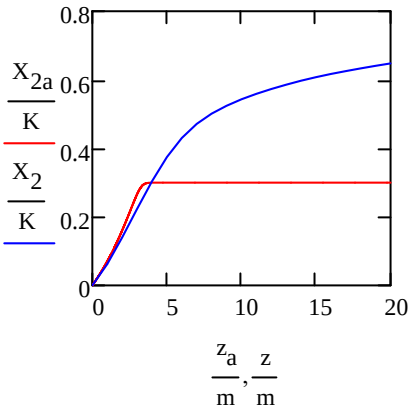
$i := 1 .. N$

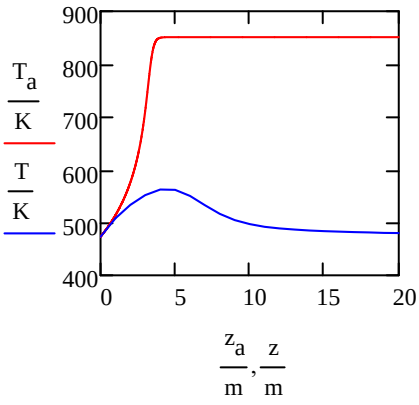
$z_{a_i} := i\cdot\Delta z_a$

$$\begin{pmatrix} X1a_i \\ X2a_i \\ \alpha a_i \end{pmatrix} := \begin{pmatrix} X1a_{i-1} \\ X2a_{i-1} \\ \alpha a_{i-1} \end{pmatrix} + \Delta z_a\cdot \begin{bmatrix} dX1\left[T_m\left[\alpha a_{i-1}\cdot(W), X1a_{i-1}, X2a_{i-1}\right], X1a_{i-1}, X2a_{i-1}\right] \\ dX2\left[T_m\left[\alpha a_{i-1}\cdot(W), X1a_{i-1}, X2a_{i-1}\right], X1a_{i-1}, X2a_{i-1}\right] \\ d\alpha\left[T_m\left[\alpha a_{i-1}\cdot(W), X1a_{i-1}, X2a_{i-1}\right], X1a_{i-1}, X2a_{i-1}\right]\cdot\left(\frac{1}{W}\right) \end{bmatrix}$$

$i := 0 .. N \qquad \alpha a := \alpha a\cdot W \qquad T_{a_i} := T_m\left(\alpha a_i, X1a_i, X2a_i\right)$

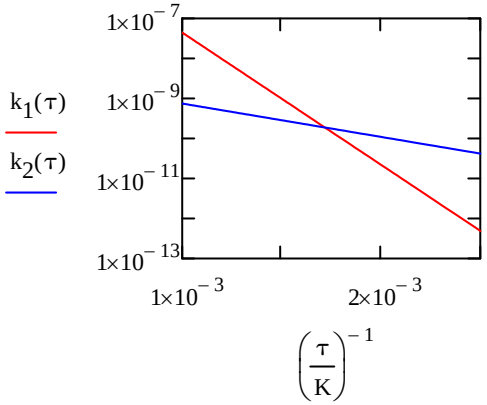


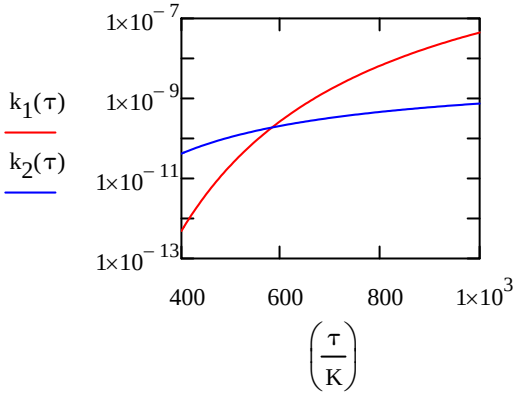


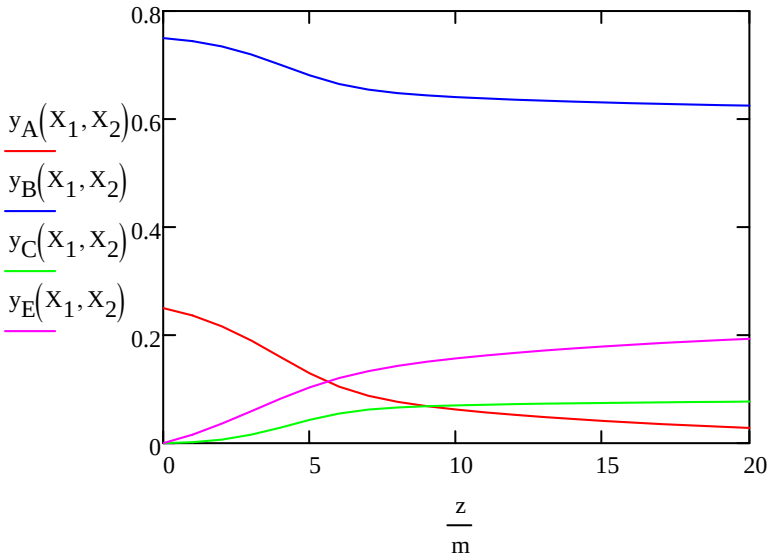


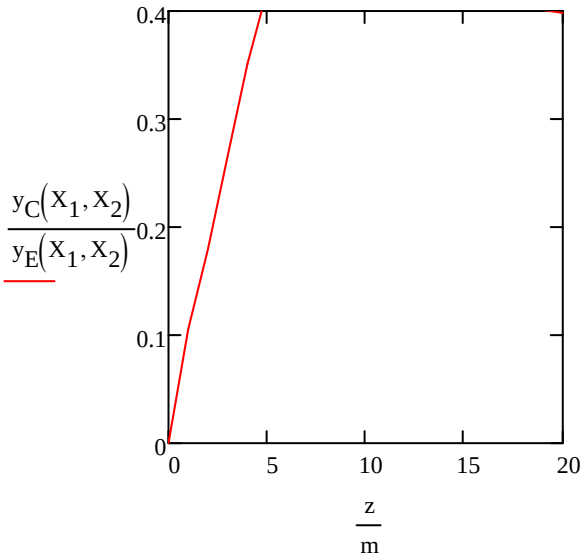
$\tau := 400\cdot K, 405\cdot K .. 1000\cdot K$

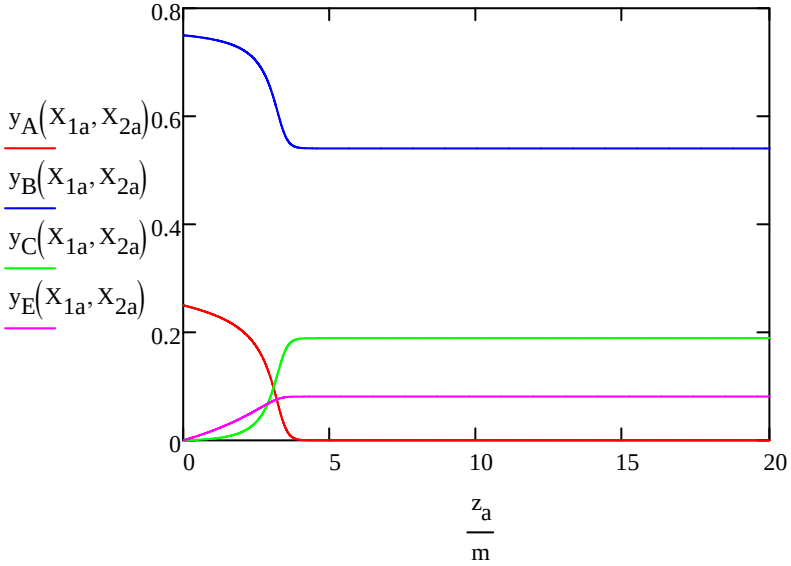
$$y_C(X_1, X_2) := \frac{n_{A0}\cdot X_1}{n_0 - n_{A0}\cdot X_2} \qquad y_E(X_1, X_2) := \frac{n_{A0}\cdot X_2}{n_0 - n_{A0}\cdot X_2}$$

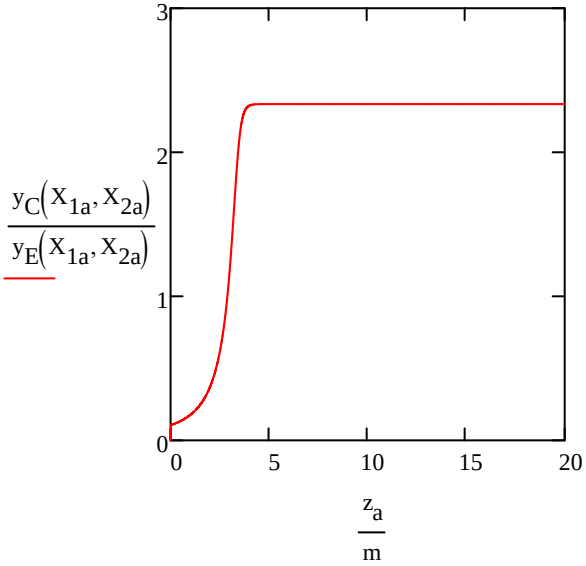





$y_A(x_1, x_2)$
$y_B(x_1, x_2)$
$y_C(x_1, x_2)$
$y_E(x_1, x_2)$
0.8
0.6
0.4
0.2
0
0
5
10
15
20
z
m


$\frac{y_C(x_1, x_2)}{y_E(x_1, x_2)}$
0.4
0.3
0.2
0.1
0
0
5
10
15
20
z
m


$y_A(x_{1a}, x_{2a})$
$y_B(x_{1a}, x_{2a})$
$y_C(x_{1a}, x_{2a})$
$y_E(x_{1a}, x_{2a})$
0.8
0.6
0.4
0.2
0
0
5
10
15
20
z_a
m


$\frac{y_C(x_{1a}, x_{2a})}{y_E(x_{1a}, x_{2a})}$
3
2
1
0
0
5
10
15
20
z_a
m

$i := 0, 1000 .. 20000$ ATTENZIONE! Qui i calcoli sono fatti con Δz = 1 mm e i risultati sono dati ogni metro di PFR

z_{a_i} =		X_{1a_i} =	X_{2a_i} =	αa_i =		T_{a_i} =		$-r_1\left(T_{a_i}, X_{1a_i}, X_{2a_i}\right)$ =		$-r_2\left(T_{a_i}, X_{1a_i}, X_{2a_i}\right)$ =	
0	·m	0.0000	0.0000	0	W	473.15	·K	0.0694	$\cdot\frac{mol}{m^3 \cdot s}$	0.6591	$\cdot\frac{mol}{m^3 \cdot s}$
1		0.0125	0.0704	308.035		513.871		0.2295		0.8399	
2		0.0595	0.1604	775.988		576.01		0.9626		1.0670	
3		0.3148	0.2658	$1.805 \cdot 10^3$		712.366		5.9692		0.9986	
4		0.6968	0.2998	$2.854 \cdot 10^3$		849.782		0.2320		0.0107	
5		0.7001	0.2999	$2.863 \cdot 10^3$		850.881		$2.7291 \cdot 10^{-4}$		$1.2438 \cdot 10^{-5}$	
6		0.7001	0.2999	$2.863 \cdot 10^3$		850.882		$3.1481 \cdot 10^{-7}$		$1.4347 \cdot 10^{-8}$	
7		0.7001	0.2999	$2.863 \cdot 10^3$		850.882		$3.6312 \cdot 10^{-10}$		$1.6549 \cdot 10^{-11}$	
8		0.7001	0.2999	$2.863 \cdot 10^3$		850.882		$5.7397 \cdot 10^{-13}$		$2.6158 \cdot 10^{-14}$	
9		0.7001	0.2999	$2.863 \cdot 10^3$		850.882		$5.7397 \cdot 10^{-13}$		$2.6158 \cdot 10^{-14}$	
10		0.7001	0.2999	$2.863 \cdot 10^3$		850.882		$5.7397 \cdot 10^{-13}$		$2.6158 \cdot 10^{-14}$	
11		0.7001	0.2999	$2.863 \cdot 10^3$		850.882		$5.7397 \cdot 10^{-13}$		$2.6158 \cdot 10^{-14}$	
12		0.7001	0.2999	$2.863 \cdot 10^3$		850.882		$5.7397 \cdot 10^{-13}$		$2.6158 \cdot 10^{-14}$	
13		0.7001	0.2999	$2.863 \cdot 10^3$		850.882		$5.7397 \cdot 10^{-13}$		$2.6158 \cdot 10^{-14}$	
14		0.7001	0.2999	$2.863 \cdot 10^3$		850.882		$5.7397 \cdot 10^{-13}$		$2.6158 \cdot 10^{-14}$	
15		0.7001	0.2999	$2.863 \cdot 10^3$		850.882		$5.7397 \cdot 10^{-13}$		$2.6158 \cdot 10^{-14}$	
16		0.7001	0.2999	$2.863 \cdot 10^3$		850.882		$5.7397 \cdot 10^{-13}$		$2.6158 \cdot 10^{-14}$	
17		0.7001	0.2999	$2.863 \cdot 10^3$		850.882		$5.7397 \cdot 10^{-13}$		$2.6158 \cdot 10^{-14}$	
18		0.7001	0.2999	$2.863 \cdot 10^3$		850.882		$5.7397 \cdot 10^{-13}$		$2.6158 \cdot 10^{-14}$	
19		0.7001	0.2999	$2.863 \cdot 10^3$		850.882		$5.7397 \cdot 10^{-13}$		$2.6158 \cdot 10^{-14}$	
20		0.7001	0.2999	$2.863 \cdot 10^3$		850.882		$5.7397 \cdot 10^{-13}$		$2.6158 \cdot 10^{-14}$	

$i := 0, 1 .. 15$ Invece questi sono i primi quindici punti con Δz = 1 mm.

z_{a_i} =		X_{1a_i} =	X_{2a_i} =	αa_i =		T_{a_i} =		$-r_1\left(T_{a_i}, X_{1a_i}, X_{2a_i}\right)$ =		$-r_2\left(T_{a_i}, X_{1a_i}, X_{2a_i}\right)$ =	
0	·mm	0.00	0.00	0	W	473.15	·K	0.0694	$\cdot\frac{mol}{m^3 \cdot s}$	0.6591	$\cdot\frac{mol}{m^3 \cdot s}$
1		$6.56 \cdot 10^{-6}$	$6.23 \cdot 10^{-5}$	0.262		473.185		0.0695		0.6592	
2		$1.31 \cdot 10^{-5}$	$1.25 \cdot 10^{-4}$	0.524		473.219		0.0696		0.6594	
3		$1.97 \cdot 10^{-5}$	$1.87 \cdot 10^{-4}$	0.786		473.254		0.0697		0.6596	
4		$2.63 \cdot 10^{-5}$	$2.49 \cdot 10^{-4}$	1.048		473.288		0.0697		0.6597	
5		$3.29 \cdot 10^{-5}$	$3.12 \cdot 10^{-4}$	1.31		473.323		0.0698		0.6599	
6		$3.95 \cdot 10^{-5}$	$3.74 \cdot 10^{-4}$	1.572		473.357		0.0699		0.6600	
7		$4.61 \cdot 10^{-5}$	$4.36 \cdot 10^{-4}$	1.834		473.392		0.0700		0.6602	
8		$5.27 \cdot 10^{-5}$	$4.99 \cdot 10^{-4}$	2.097		473.426		0.0700		0.6603	
9		$5.93 \cdot 10^{-5}$	$5.61 \cdot 10^{-4}$	2.359		473.461		0.0701		0.6605	
10		$6.60 \cdot 10^{-5}$	$6.24 \cdot 10^{-4}$	2.622		473.496		0.0702		0.6606	
11		$7.26 \cdot 10^{-5}$	$6.86 \cdot 10^{-4}$	2.884		473.53		0.0703		0.6608	
12		$7.92 \cdot 10^{-5}$	$7.49 \cdot 10^{-4}$	3.147		473.565		0.0704		0.6610	
13		$8.59 \cdot 10^{-5}$	$8.11 \cdot 10^{-4}$	3.41		473.6		0.0704		0.6611	
14		$9.26 \cdot 10^{-5}$	$8.74 \cdot 10^{-4}$	3.672		473.634		0.0705		0.6613	
15		$9.92 \cdot 10^{-5}$	$9.36 \cdot 10^{-4}$	3.935		473.669		0.0706		0.6614	