TLS-MC : ThermoLuminescence Simulation in MathCad

Last revised: 2015-01-27

Helper functions

========== Definition of the system ==========

$$\text{ElectronTraps} := \begin{pmatrix} \text{"110°C TL"} & \text{"230°C TL"} & \text{"OSL-F"} & \text{"OSL-M"} & \text{"Deep"} \\ 1.5\cdot10^{7} & 10^{7} & 10^{9} & 2.5\cdot10^{8} & 5\cdot10^{10} \\ 0.97 & 1.55 & 1.7 & 1.72 & 2 \\ 5\cdot10^{12} & 5\cdot10^{14} & 5\cdot10^{13} & 5\cdot10^{14} & 10^{10} \\ 10^{-8} & 10^{-8} & 10^{-9} & 5\cdot10^{-10} & 10^{-10} \end{pmatrix}$$

$$\text{HoleTraps} := \begin{pmatrix} \text{"R1"} & \text{"R2"} & \text{"L"} & \text{"K"} \\ 3\cdot10^{8} & 10^{10} & 10^{11} & 5\cdot10^{9} \\ 1.43 & 1.75 & 5 & 5 \\ 5\cdot10^{13} & 5\cdot10^{14} & 10^{13} & 10^{13} \\ 5\cdot10^{-7} & 10^{-9} & 10^{-9} & 10^{-10} \\ 5\cdot10^{-9} & 5\cdot10^{-10} & 10^{-10} & 10^{-10} \end{pmatrix}$$

Each column represents data for single trap in the
Row 1. Name
Row 2. Concentration (L^{-3})
Row 3. Trap depth (eV)
Row 4. Frequency factor (T^{-1})
Row 5. Trapping rate (T^{-1} L^{3})
Row 6. Recombination rate (T^{-1} L^{3}). Optional (defa

Note that only energy and temperature units are fi
volume (L^{3}) units can be arbitrary, subject to interp
thermoluminescence the time unit might be a secc
millisecond. All numerical values must be in coher

Processing

Temperature-dependent luminescence efficiency: $\eta(T) := \frac{1}{1 + 2.8 \cdot 10^{7} \cdot \exp\left(-\frac{0.64}{k_B \cdot T}\right)}$

The recombination center responsible for the observed glow: RecombCenter := htrap("L")
(etrap(id) **for electron traps and** htrap(id) **for hole traps, using either name or index as id)**

Direct band-to-band recombination rate (T^{-1} L^{3}): DirectRecombRate := 0

Initial populations (after calculation, check the variable Final **for the final state):**

$$\text{Init} := \left[\begin{pmatrix} 0.296311134994926 \\ 69.72334235328006 \\ 4.418527221299608 \times 10^{5} \\ 2.073367896235399 \times 10^{3} \\ 3.823730118573273 \times 10^{10} \end{pmatrix} \begin{pmatrix} 2.217810330725511 \times 10^{-6} \\ 2.819651330159122 \times 10^{-5} \\ 3.797932597892948 \times 10^{10} \\ 2.586661110506791 \times 10^{8} \end{pmatrix} \quad 2.469081380913029 \times 10^{5} \quad 4.46844571384298 \times 10^{-6}\right]$$

1. el
2. el
3. el
4. el

========== Excitation and temperature vs time ==========

Excitation rate (T^{-1} L^{-3}) as a function of time: Excitation := PWCF((0 LEVEL 10^7) (10 LEVEL 0))

Temperature (K) as a function of time: Temperature := PWCF((0 DEFAULT 293) (15 RAMP 5))

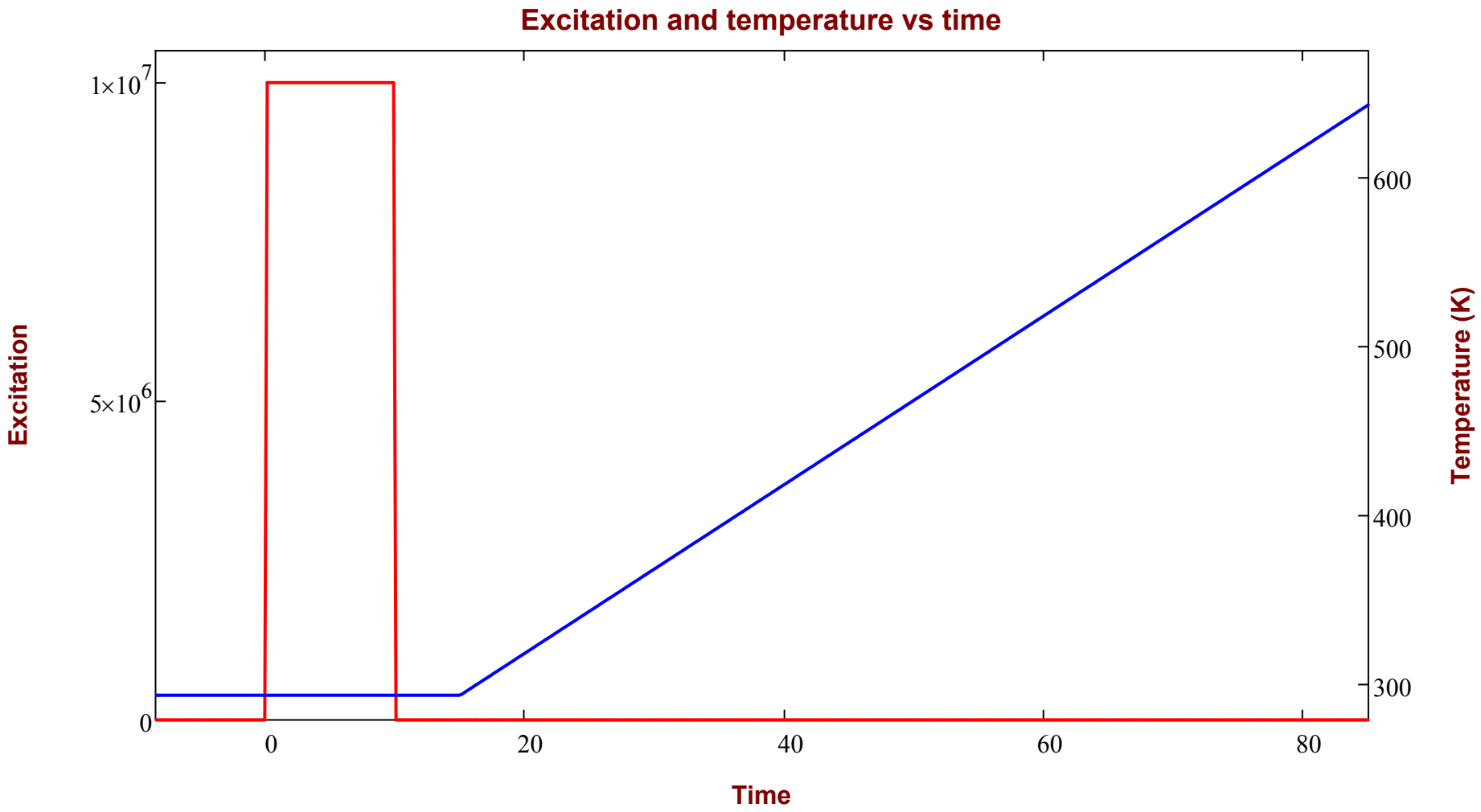
Time span in seconds: TimeSpan := 85

Time step in seconds: TimeStep := 0.1

Processing

Defining piecewise co
DEFAULT The
LEVEL Cons
RAMP Cons
DECAY Expo
Click here for more d

If the definitions are c


Excitation and temperature vs time
1×10^7
5×10^6
0
Excitation
0
20
40
60
80
Time
600
500
400
300
Temperature (K)

========== Numerical method ==========

ODE integration method: OdeSolver := BDF

Possible choices (copy-paste):

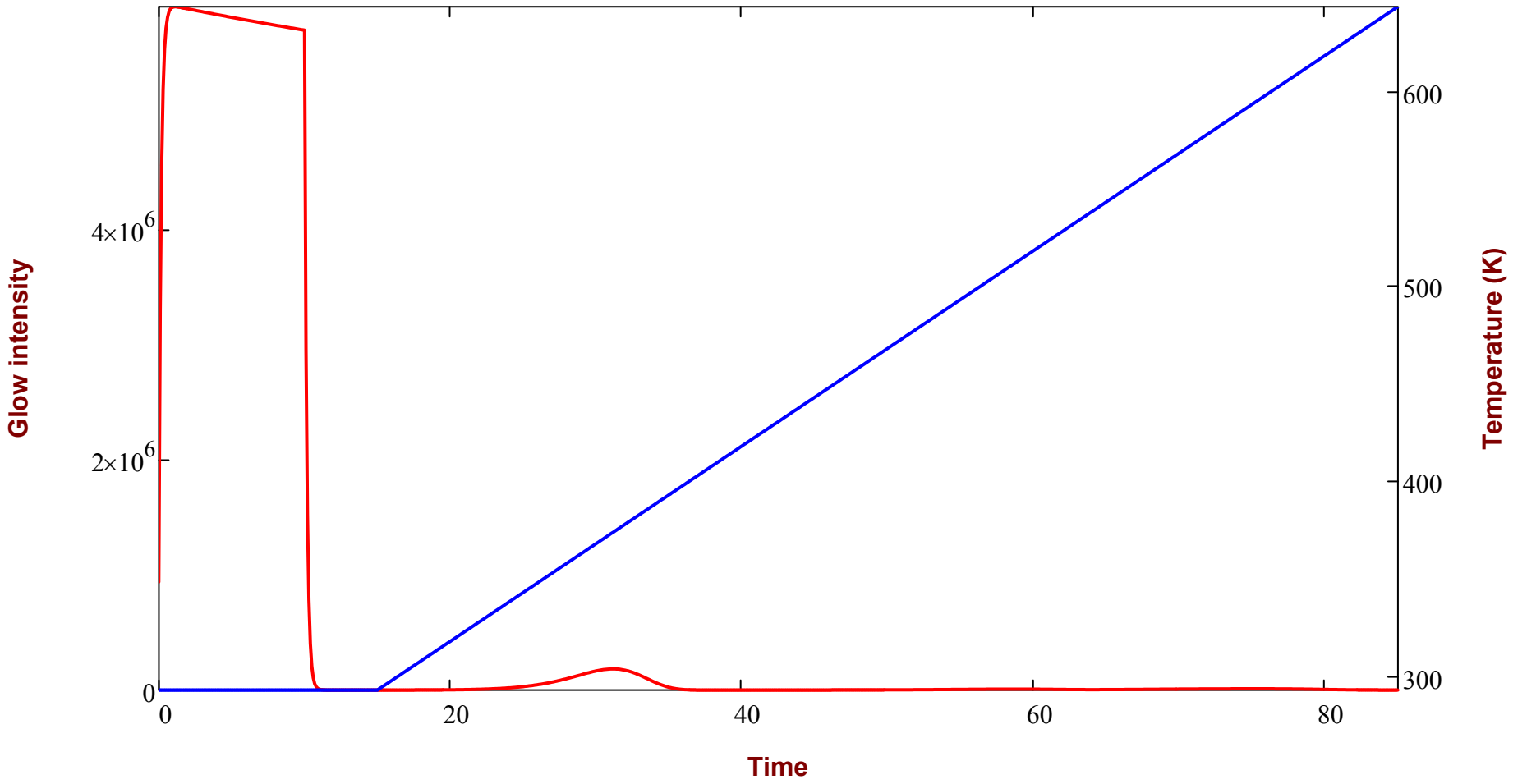
1. RK3fixed **(3th order Runge-Kutta with fixed step size)**
2. RK4fixed **(4th order Runge-Kutta with fixed step size)**
3. RK4adapt **(4th order Runge-Kutta with adaptive step size)**
4. Bulstoer **(Bulirsch-Stoer method)**
5. Adams **(Adams methods)**
6. BDF **(backward differentiation formula method)**

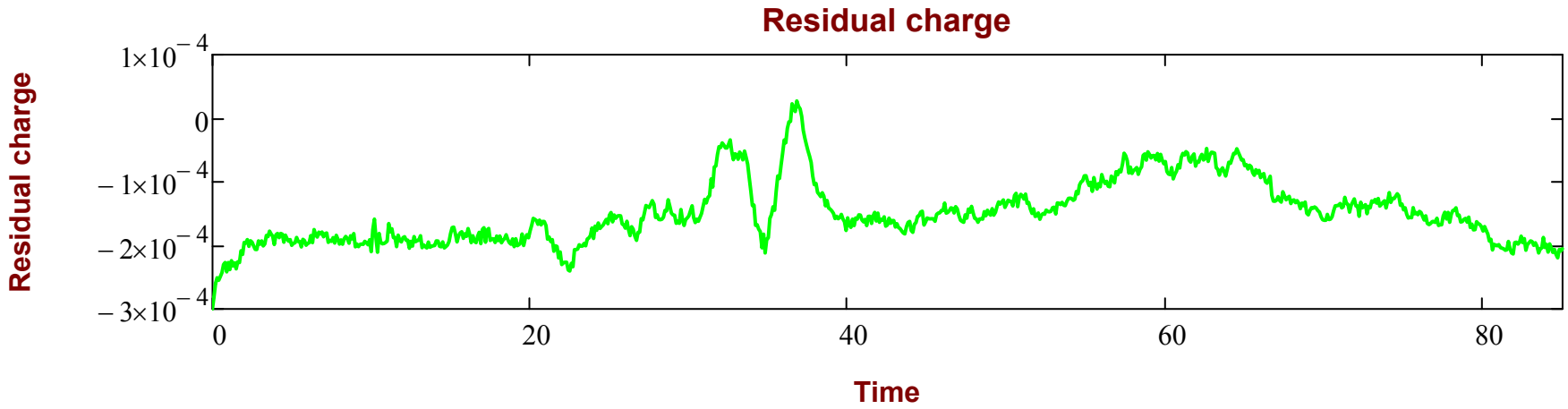
In some cases a scaling of the population variables may be needed to improve the stability of the numerical process. ScaleFactor := 10^{-5}

Processing

========== Glow intensity vs time ==========

Rescale := 1





Total number of emitted photons per unit volume: $\text{TotalEmittedPhotons} = 5.99 \times 10^{7}$

In order to copy the final state back to the initial state for the next run, very high accuracy must be preserved, otherwise the existing accuracy of charge neutrality will be lost.

$$\text{Final} = \left[\begin{pmatrix} 0.023727159151325 \\ 5.561800555739979 \\ 1.476903236727602 \times 10^{4} \\ 153.06417522618744 \\ 3.82601228115236 \times 10^{10} \end{pmatrix} \begin{pmatrix} 1.817201884654544 \times 10^{-8} \\ 2.241444637823721 \times 10^{-7} \\ 3.800126154543823 \times 10^{10} \\ 2.58895960549744 \times 10^{8} \end{pmatrix} \quad 1.976678250815725 \times 10^{4} \quad 3.655407077964183 \times 10^{-8} \right]$$

$\text{WRITEPRN}(\text{"glow-vs-time.txt"}) := \text{augment}(\text{Time}, \text{Temp}, \text{Glow})$

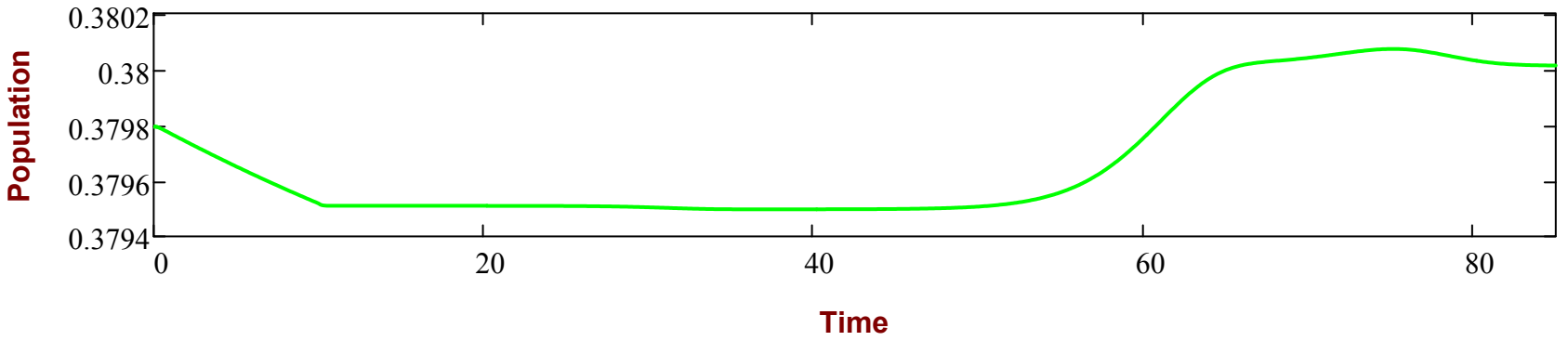
========== Population vs time ==========

Name of the trap or index of population variable: Index := htrap("L")

(use etrap(id) **for electron traps,** htrap(id) **for hole traps,** cond **for conduction band,** valence **for valence band and** recomb **for r**

Relative := 1

Processing



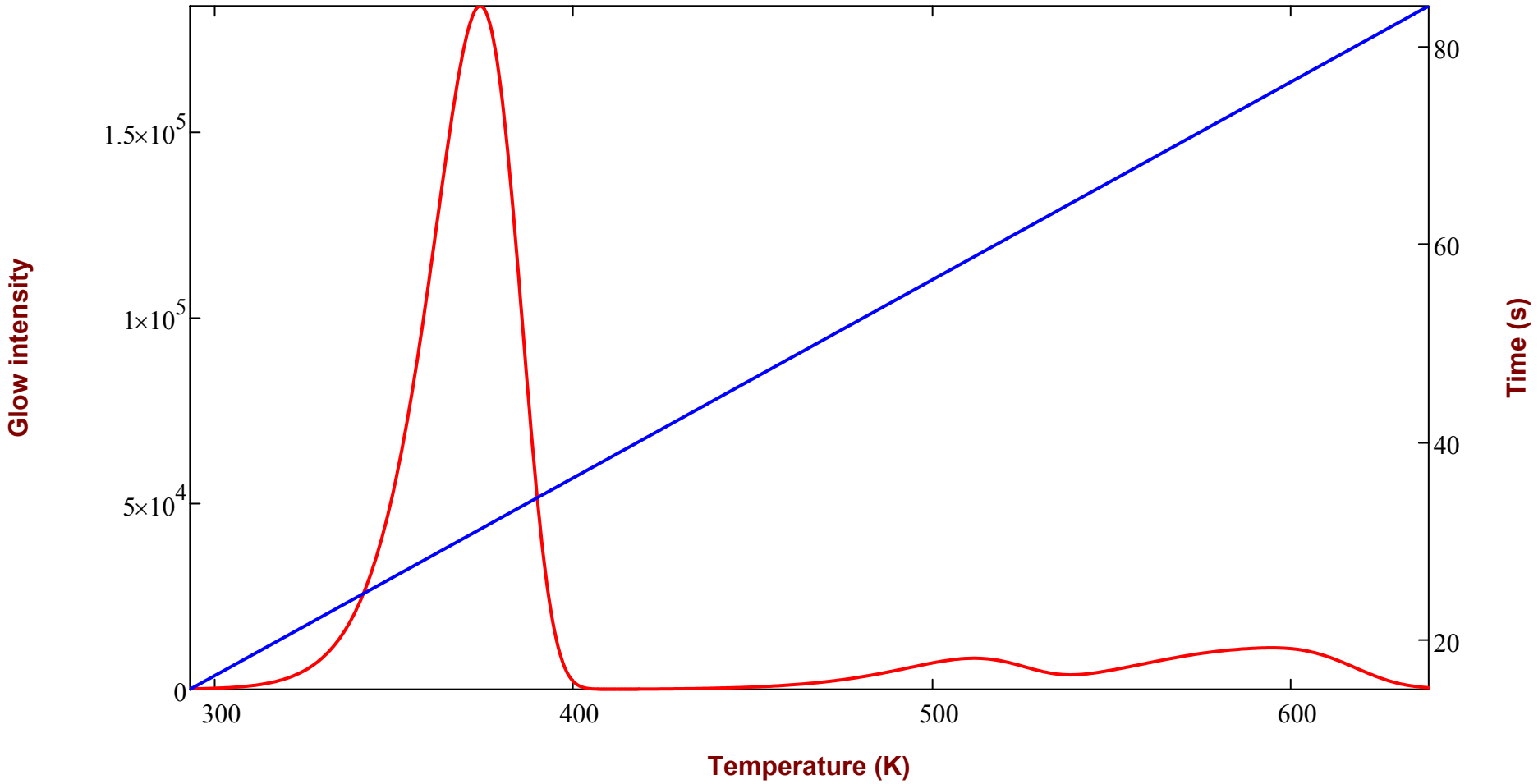
WRITEPRN("filling-vs-time.txt") := augment(Time, Filling, ResidualCharge)

WRITEPRN("popul-vs-time.txt") := augment(Time, Popul, ResidualCharge)

================ Glow intensity vs temperature ================

Time range for extracting the TL glow curve: TimeRange := (15 84)

Processing



```
WRITEPRN("glow-vs-temp.txt") := augment(Temp,Glow)
```

========== End of Program ==========