

1.The Semenov Model

<http://demonstrations.wolfram.com/TheSemenovModel/>

Semenov developed a model that describes the thermal ignition phenomenon quantitatively

Denote the

$x_1 = \gamma \qquad x_2 = T \qquad \varepsilon := 0.15$

where T is a dimensionless temperature, γ depends on the overall heat transfer coefficient, and ε depends on the activation energy

The dimensionles equation

$f_1 := e^{-\frac{1}{\varepsilon \cdot x_2}} - x_1 \cdot (x_2 - 1) = 0$

Координаты начальных точек

$X0_1 := 0.1$
 $X0_2 := \text{solve}\left(e^{-\frac{1}{\varepsilon \cdot T}} - X0_1 \cdot (T - 1) = 0, T, 0, 15\right)$

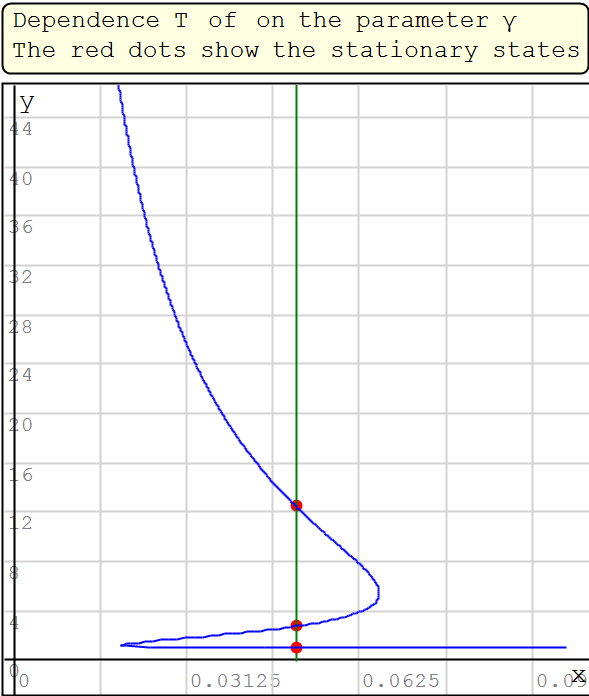
⊞—Dragilev's Method

$tmin := 0 \qquad tmax := -48 \qquad \Delta t := -0.06 \qquad N := \frac{tmax}{\Delta t} \qquad N = 800$

$B := D(X0, tmin, tmax, N) \qquad \gamma(t) := 0.021 + 0.0025 \cdot t$

$T(t) := \left| \begin{array}{l} \text{root} := \text{solve}\left(e^{-\frac{1}{\varepsilon \cdot Y}} - \gamma(t) \cdot (Y - 1) = 0, Y, 0, 50\right) \\ T := \text{if } t > 18.8 \\ \qquad \text{stack}(\text{root}, 100, 100) \\ \qquad \text{else} \\ \qquad \text{root} \end{array} \right|$

$\tau := 0 \dots 28$



2. Continuously Stirred Tank Reactor

<http://demonstrations.wolfram.com/ContinuouslyStirredTankReactorUsingArcLengthParameter/>

x_1 -dimensionless concentration, x_2 -dimensionless temperature, Da -Damköhler number,
 γ -dimensionless activation energy, β -dimensionless heat transfer coefficient

$B := 10$ $Da := 0.03084$ $\gamma := 20$ $T_0 := -5$

Denote the

$x_1 = x$ $x_2 = T$ $x_3 = Da$

Координаты начальных точек

$X_{0_1} := 0.004$ $X_{0_2} := -1.85$ $X_{0_3} := 0.03084$

$t_{\min} := 0$ $t_{\max} := -9.8$ $\Delta t := -0.2$ $N := \frac{t_{\max}}{\Delta t}$

The dimensionless equations

$$\varphi := -x_2 + B \cdot x_3 \cdot \left(1 - x_1\right) \cdot e^{\frac{x_2}{1 + \frac{x_2}{\gamma}}}$$

$$f_1 := -x_1 + x_3 \cdot \left(1 - x_1\right) \cdot e^{\frac{x_2}{1 + \frac{x_2}{\gamma}}} = 0$$

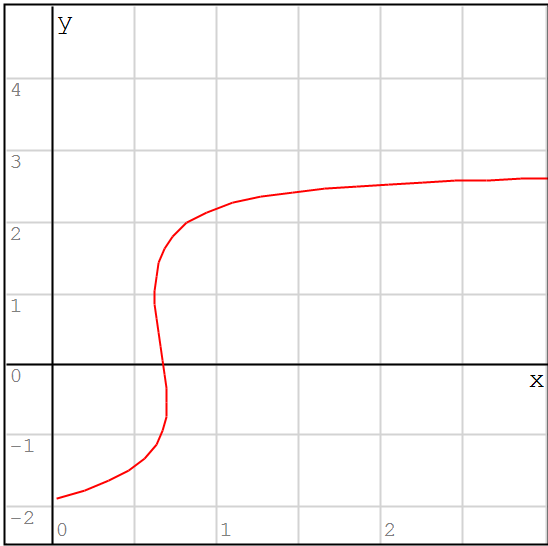
$t_{\text{start}} := 6$ $t_{\text{end}} := 30$

for $i \in t_{\text{start}} \dots t_{\text{end}}$

$$\left| \begin{array}{l} \beta_i := 0.2 + 0.04 \cdot i \\ f_2 := \varphi - \beta_i \cdot x_2 \\ K_i := D(X_0, t_{\min}, t_{\max}, N) \end{array} \right.$$

$\tau := t_{\text{start}} \dots 2 \cdot t_{\text{end}} - t_{\text{start}}$

Dependence T of on the parameter Da .
By increasing the heat transfer
coefficient the temperature drops



$X0_1 := 1.496446999$

$X0_2 := -0.9574371296$

$X0_3 := 0$