# Chemical Kinetics II

EDU 109

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## Review of Rate Laws

Simple First Order Reactions

$A \xrightarrow{k} B \qquad A_o = a,\ B_o = 0$

$$\frac{dA}{dt} = -kA \qquad A = ae^{-kt}$$

$$\frac{dB}{dt} = kA \qquad B = a\left(1 - e^{-kt}\right)$$

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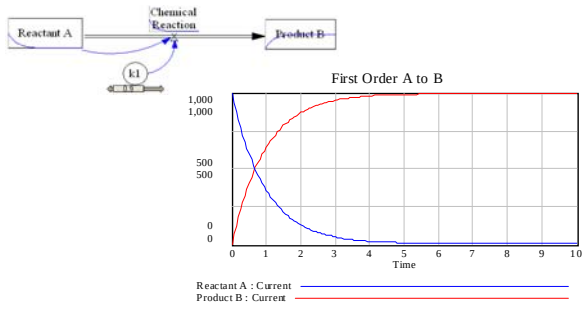
## Graphical Interface Differential Equation Solvers

Vensim PLE (www.vensim.com)

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## Review of Rate Laws

Consecutive First Order Reactions

$A \xrightarrow{k_1} B \xrightarrow{k_2} C$ $\quad A_o = a, B_o = C_o = 0$

$$\frac{dA}{dt} = -kA \qquad A = ae^{-kt}$$

$$\frac{dB}{dt} = k_1 A - k_2 B \qquad B = \frac{ak_1}{k_2 - k_1}\left(e^{-k_1 t} - e^{-k_2 t}\right)$$

$$\frac{dC}{dt} = k_2 B \qquad C = a\left(1 - \frac{k_2 e^{-k_1 t}}{k_2 - k_1} - \frac{k_1 e^{-k_2 t}}{k_1 - k_2}\right)$$

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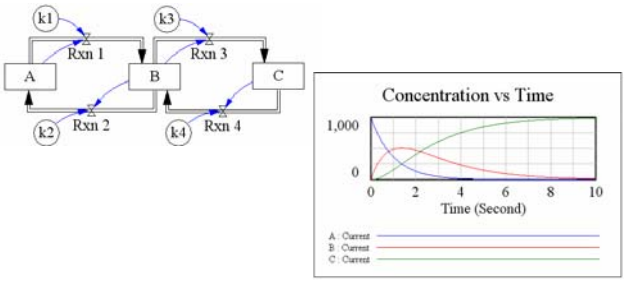
## Graphical Interface Differential Equation Solvers

A ⇄ B ⇄ C

First Order and Reversible First Order

Consecutive First Order and Reversible First Order

(Disequilibrium, Transient Equilibrium, Secular Equilibrium)

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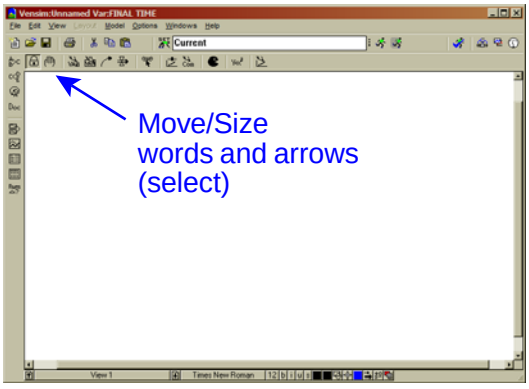
## Vensim PLE Interface

Initial Window

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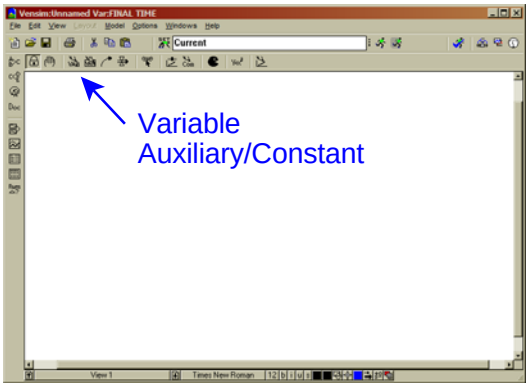
## Vensim PLE Interface

Variables

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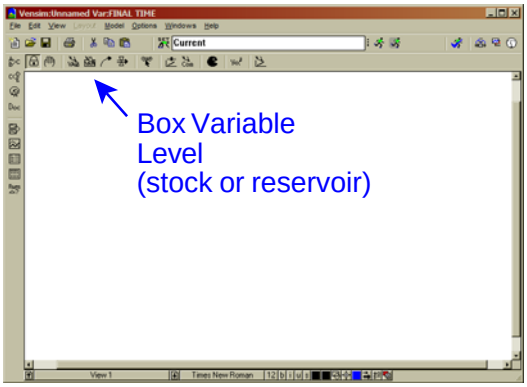
## Vensim PLE Interface

Variables

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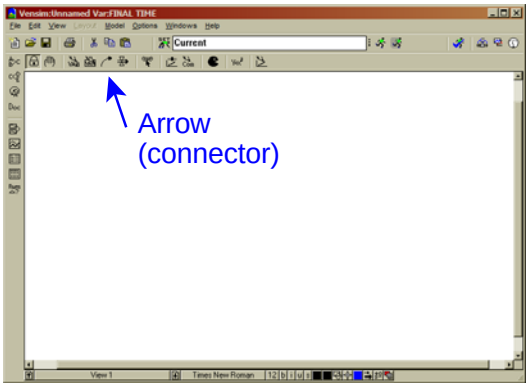
## Vensim PLE Interface

Arrow

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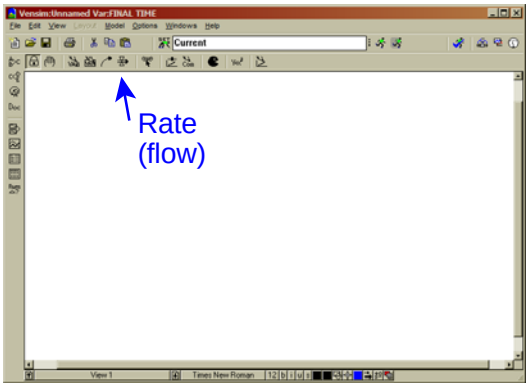
## Vensim PLE Interface

Rate

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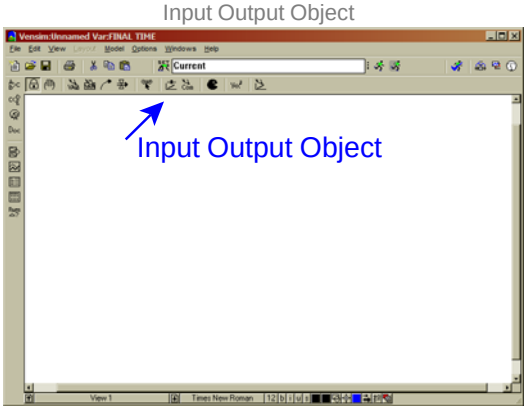
## Vensim PLE Interface

Input Output Object

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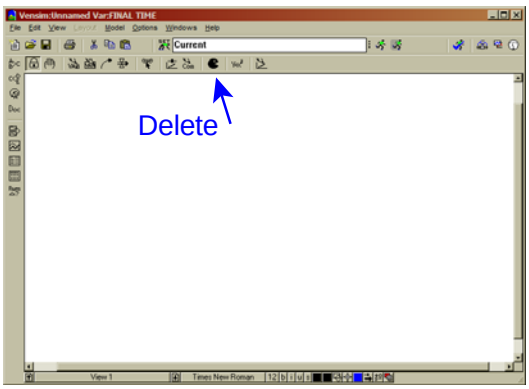
## Vensim PLE Interface

Delete

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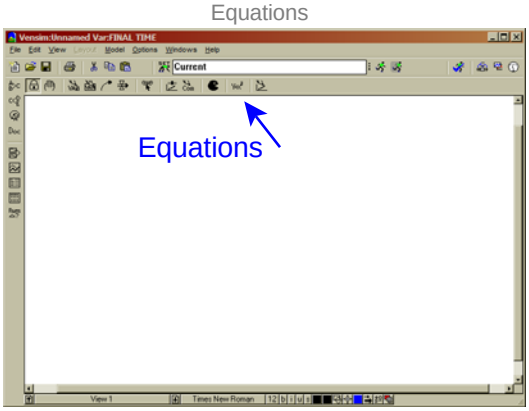
## Vensim PLE Interface

Equations

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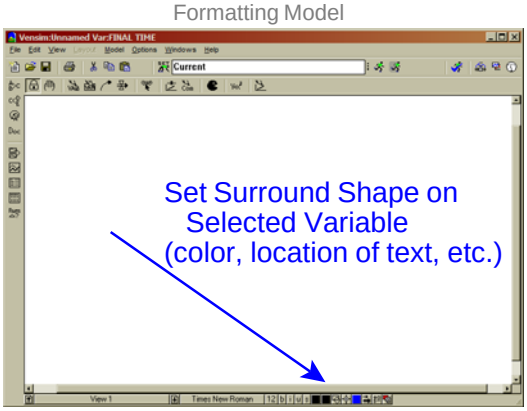
## Vensim PLE Interface

Formatting Model

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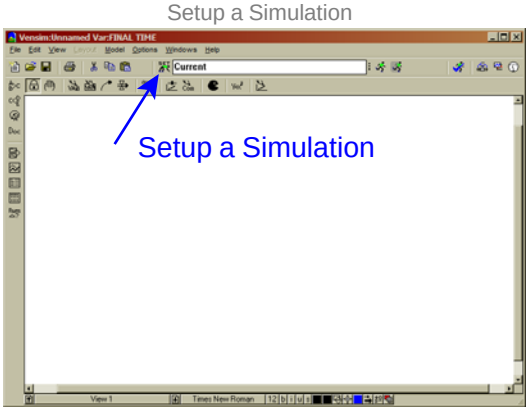
## Vensim PLE Interface

Setup a Simulation

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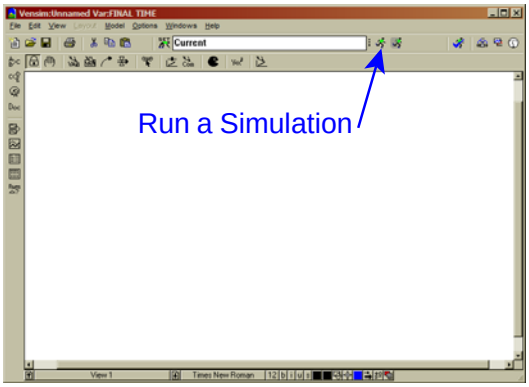
## Vensim PLE Interface

Run a Simulation

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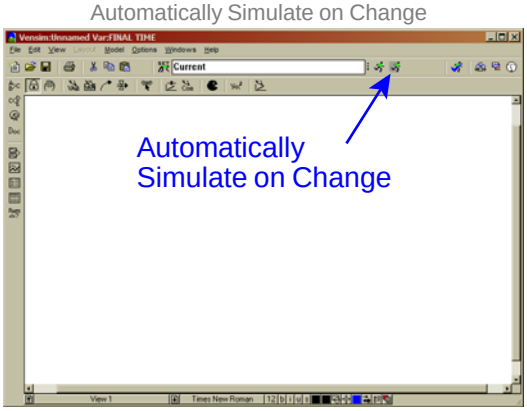
## Vensim PLE Interface

Automatically Simulate on Change

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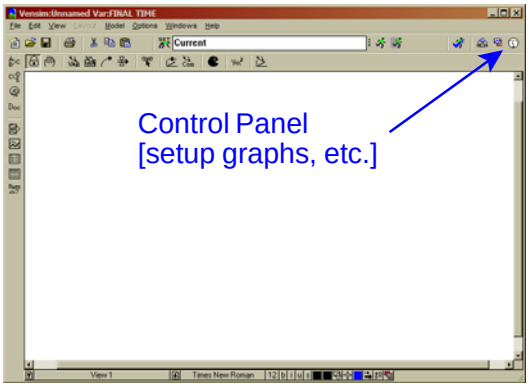
## Vensim PLE Interface

Control Panel

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