

Symbol	Definition	Value
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### 1. Constants

$k$	Boltzmann's constant	$1.3806 \times 10^{-23} \text{ J/(molec}\cdot\text{K)}$
$N_0$	Avagadro's number	$6.022 \times 10^{23}$

### 2. Simulation Variables

$N$	Number of molecules	$\sim 10^3$
$V$	Simulation cell volume	$\sim 10^{-24} \text{ m}^3$
$m$	Molecular mass	$\sim 10^{-25} \text{ kg/molec}$
$\rho$	Number density	$\sim 10^{27} \text{ molec/m}^3$
$E$	Energy (total)	$\sim 10^{-20} \text{ J/molec}$
$t$	time	$\sim 10^{-12} \text{ s}$

### 3. Model Variables

$\sigma$	Size variable	$\sim 5 \times 10^{-10} \text{ m}$
$\epsilon$	Energy variable	$\sim 10^{-21} \text{ J/molec}$
$r_b$	Bond distance	$\sim 10^{-10} \text{ m}$
$k_v$	Vibrational spring constant	$\sim 10^3 \text{ J/m}^2$