

## Documentation for the “Molecular Interactions” Series

John Mallinckrodt—Cal Poly Pomona—July 2002

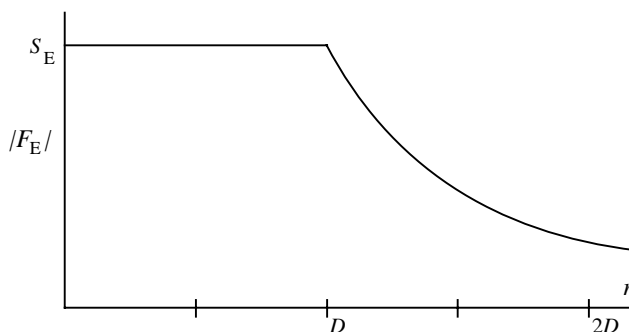
All of the modules in the “Molecular Interactions” series are derived from the basic behaviors illustrated in the primary module titled simply “Molecular Interactions.” In each one, all molecules have the same diameter and mass with the red and blue molecules carrying unit positive or negative charge (respectively) and the gray molecules being electrically neutral. The molecules interact via the superposition of a modified Coulomb force  $F_E$  and an intermolecular-type force  $F_M$ .

$$\vec{F} = (F_E + F_M)\hat{r}$$

The Coulomb force is modified to eliminate the singularity at  $r = 0$  and the numerical integration artifacts that would be the inevitable result.

After some experimentation I chose simply to apply a ceiling to the magnitude of the force at the value it attains when the molecules are “just touching”—that is, when the separation is equal to the nominal molecular diameter  $D$ . The force is given analytically by

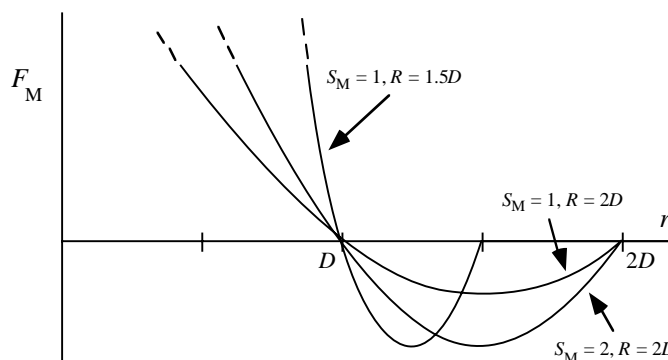
$$F_E = \frac{S_E q_1 q_2}{(\max(r/D, 1))^2}$$



The strength  $S_E$  is adjustable and the charges  $q_1$  and  $q_2$  are always  $\pm 1$  or 0 depending, as previously indicated, on the color of the molecule.

The intermolecular-type force exhibits strong repulsion at small separations and attraction at larger separations. It is modeled by a parabola that is truncated at its second zero crossing as shown in the graph. In all cases, the

intermolecular force has an equilibrium position at a separation equal to the nominal molecular diameter and the attractive region extends to  $R$  (the “range parameter”) times the diameter. The value of  $S_M$  (the “strength parameter”) is proportional to the energy required to separate two molecules starting at the equilibrium position. Thus, for smaller ranges with constant strength, the bond necessarily becomes quite a bit “stiffer.” The force is given analytically by



$$F_M = \frac{6S_M}{(R/D - 1)^3} \left[ \left( r/D - \frac{R/D + 1}{2} \right)^2 - \left( \frac{R/D - 1}{2} \right)^2 \right] \text{ if } r \leq R, \quad 0 \text{ otherwise.}$$

In some modules, the user is allowed to add and adjust the strength of a velocity-dependent drag and/or an external gravitational field.