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Using the Morse Potential to Understand Reaction Coördinates using Maple

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Abstract

The interactions employed in the "linear" reaction $A(g)+BC(g) \rightarrow AB(g) + C(g)$ in a "one dimensional world" can be used to illustrate the "reaction coördinate", using Maple, in a manner which allows students to inspect potential energy surfaces, make contour maps of those surfaces, and conceptually construct the "reaction coördinate" by tracing the local minimum path on the surface created.

Introduction

When teaching elementary kinetics to chemistry students, we often start with the pseudo reaction

$$A(g)+BC(g) \rightarrow AB(g) + C(g)$$
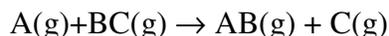
In which all three nuclei lie on a line, and the exchange shown in the equation is actually a depiction of which internuclear distances are large and which are small. Often, we then sketch a potential energy surface for this situation, which allows discussion of finding the so-called reaction coördinate, that minimal path in the A-B and B-C distances which allows us to traverse the potential from A and BC to AB and C.

Maple Code (1)

We begin with simple Maple code to generate two Morse[i] potentials

$$PE(r) = D_e (1\text{-}e^{-\alpha(r\text{-}r_e)})^2 = V(1\text{-}e^{-\alpha x})^2$$

one between nuclei B and C (PE_1) and one between nuclei A and B (PE_2). Adding these two together functionally over the domain of x_1 and x_2 and plotting them, one sees immediately the trough where both distances conform to the triple collision A-B-C. Figure 1 illustrates the potential energy surface itself, and Figure 2 illustrates the three dimensional contour map of the same surface. Students can rotate these plots on their own worksheets to see transparently what is happening. They can tweak the various constants, lo, V_1, V_2, etc., searching for clearer or better defined illustrations of the concept.

```
with(plots);
lo := -0.8;
V1 := 20; V2 := 21;alpha1 := 1; alpha2 := 1.1;
PE1 := V1*(1-exp(-alpha1*x1))^2;
PE2 := V2*(1-exp(-alpha2*x2))^2;
PotE := PE1+PE2;

plot3d(PotE,x1=lo..6,x2=lo..6,axes=boxed,labels=[`x1`,`x2`,`PE`]
);
```

```
contourplot3d(PE1+PE2,x1=lo..6,x2=lo..6,axes=boxed,contours=30,l
abels=[`x1`,`x2`,`PE`]);
```
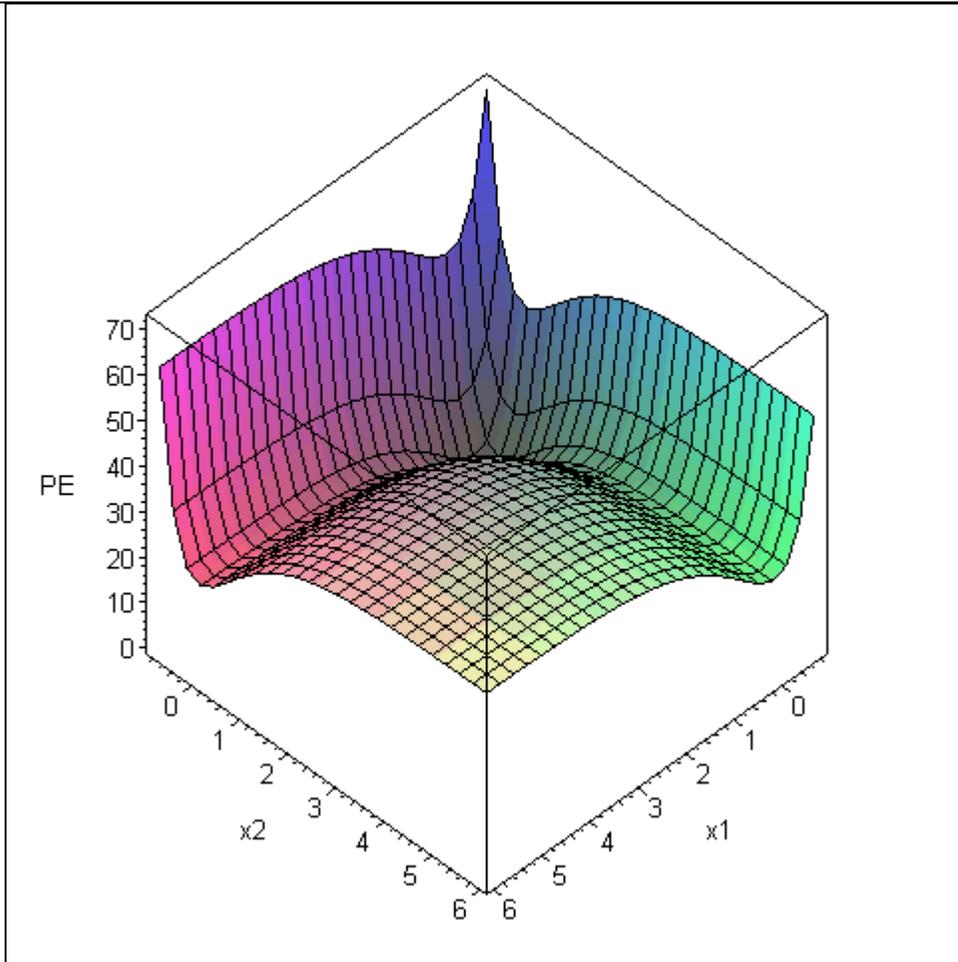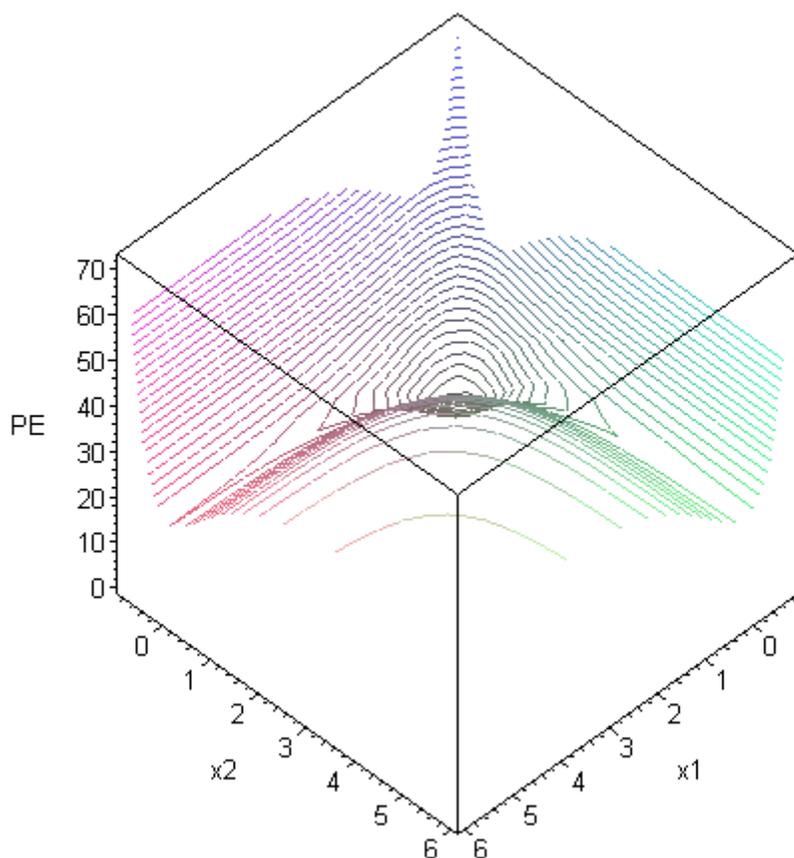

Figure 1 The pseudo 3-dimensional potential energy surface

The potential energy is being plotting in a pseudo 3-dimensional form, since x_1 and x_2 are not orthogonal coördinate axes. Each corresponds to a relative distance, so that the zero of each is chosen at the expected internuclear distance of the diatomic species.


Figure 2 The contour map (in pseudo 3D) corresponding to Figure 1

Maple Code (2)

We can add a repulsive potential energy to the two Morse potentials, to simulate an activation barrier. The form need only create the "bump" we need in the place we need, i.e., something of the form $Ae^{-\beta(x_1-x_2)^2}$ will do. The parameters A and β can be adjusted for esthetic

reasons. We an obtain an equivalent of Figure 1 (see Figure 3)
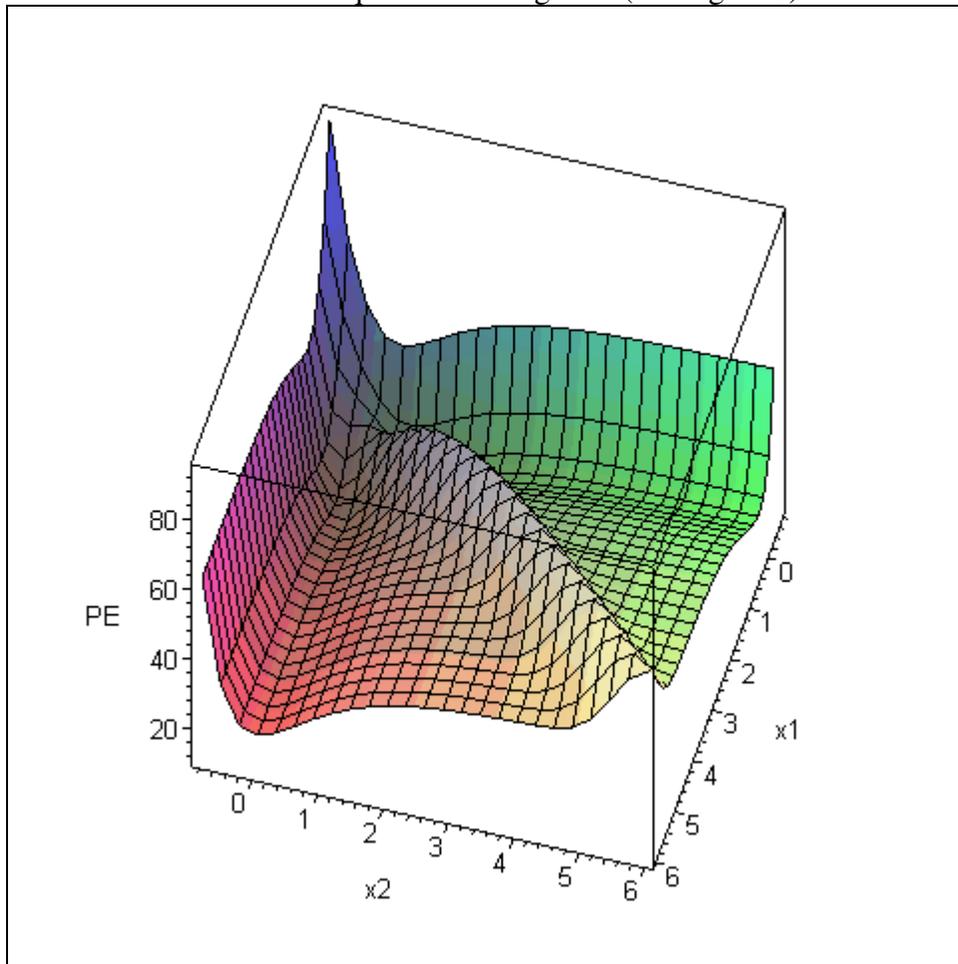
Figure 3 The potential Energy function with an extra repulsive term

and a "2-dimensional" contour map of this new potential energy surface
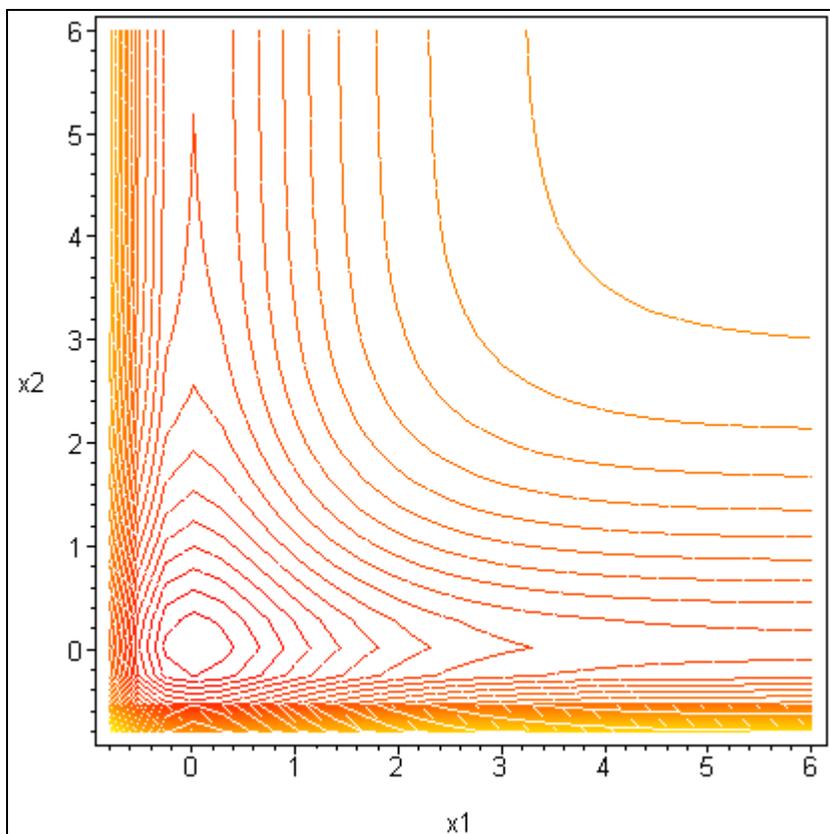
Figure 4 A contour map of Figure 3's potential energy surface

(see Figure 3) as Figure 4. It is a simple exercise to "fiddle" with the various parameters in the three potential energy functions to see "what is going on".

Discussion

The use of symbolic mathematical programs to illustrate concepts which words fail at describing is worth pursuing in any context where the mathematics obscures the understanding. The simplistic introduction of the reaction coördinate and the "activation barrier" becomes more concrete with the introduction of a plotting scheme which allows students to "see" the concept in "concrete" terms. In this context, the discussion of activation barriers as well as exothermicity (and endothermicity") follows easily, and can be grasped better.

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[i] P. M. Morse, *Phys. Rev.* 1929, **34**, 57-64.