PARTICLE MODELLING OF COMBUSTION

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by

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ABSTRACT

Combustion is simulated by a molecular type model using classical molecular type interaction formulas. Supercomputer examples which emphasize turbulent motion are described and discussed.

* Computations performed at the University of Texas Center for High Performance Computation
INTRODUCTION

Interest in combustion is as old as man's acquaintance with fire. However, it is only of more recent origin that chemists, physicists, mathematicians, and engineers have made extensive analytical and experimental studies of the subject. Of late, environmentalists have become additional interested participants.

Current theories of combustion are primarily continuum theories, even though it is understood clearly that combustion is a noncontinuum, molecular phenomenon (see, e.g., refs. [4], [6], [7], and the numerous references contained therein). The equations studied are relatively small systems of differential equations which relate the reaction of a physical system to the release of chemical energy. Major areas of inquiry relate to fuels, ignition, heat transfer, mass transfer, flames, explosions, equations of state, enthalpy, equilibrium, turbulence and conservation laws.

With the advent of modern computer technology, there has, however, been a growing interest in molecular modelling [3], [5] and particle (molecular type) modelling [1], [2]. The equations of these models are large systems of nonlinear, ordinary differential equations which incorporate or approximate the dynamics of classical molecular mechanics. These systems have to be solved numerically [2]. Our purposes in this paper are to demonstrate, qualitatively, the feasibility of simulating combustion phenomena by this new type of modelling and to derive intuition for later quantitative modelling.

MODEL FORMULATION.

Consider 1080 particles $P_i$, $i=1, 2, \ldots, 1080$, each of unit mass, arranged in nine rows of 120 particles each, with respective coordinates $(x(i), y(i))$ given by

- $x(1)=0.0$, $y(1)=0.0$, $x(121)=0.5$, $y(121)=0.866$
- $x(i+1)=1.0+x(i)$, $y(i+1)=y(1)$, $i=1, 2, \ldots, 119$
- $x(i+1)=1.0+x(i)$, $y(i+1)=y(121)$, $i=121, 122, \ldots, 239$
- $x(i)=x(i-240)$, $y(i)=1.732+y(i-240)$, $i=241, 242, \ldots, 1080$.

These positions are the vertices of a regular triangular grid whose basic triangular unit has edge length unity. The particles, shown in Figure 1, are bounded by a rectangular region which is 120 units long and 6.928 units high.
Initial particle velocities \( (v_x(i), v_y(i)) \) are assigned in a relatively random fashion in terms of parameters \( v \) and \( V \) as follows:

\[
\begin{align*}
  v_x(i) &= v_y(i) = v, \quad i = 1, 2, \ldots, 119 \\
  v_x(i) &= v_y(i) = v, \quad i = 121, 122, \ldots, 239 \\
  v_x(i) &= -v_y(i) = -v, \quad i = 241, 242, \ldots, 1080.
\end{align*}
\]

which are then modified by

\[
\begin{align*}
  v_x(5i) &= -v_y(4i) = v_x(4i) &= -v_y(5i) = v, \quad i = 1, 2, \ldots, 200,
\end{align*}
\]

and which are further modified by

\[
\begin{align*}
  v_x(i) &= V, \quad v_y(i) = 0, \quad \text{if } x(i) \leq 2.1.
\end{align*}
\]

The choice of \( v \) will be much smaller than that of \( V \). The particle velocities in the range \( x(i) \leq 2.1 \), which is the shaded region in Figure 2, will be chosen to simulate ignition.

We assume that any particle \( P_i \) is acted upon only by those particles \( P_j \) which are within 2 units of \( P_i \). The force of interaction will be of a local molecular type, with magnitude \( F \) given by

\[
F = -\frac{25}{r_{ij}} + \frac{25}{r_{ij}^3},
\]

in which \( r_{ij} \) is the distance between \( P_i \) and \( P_j \). When \( v \) and \( V \) have been prescribed, the motion of the system will be determined by Newtonian dynamics, with the resulting 1080 second order, nonlinear vector equations being solved numerically by the leap-frog formulas [2] with \( \Delta t = 0.0001 \).

During the simulation, the particles will fall into three distinct categories: combustion, fuel, and burned particles. Prior to ignition, all 1080 particles are assumed to be fuel particles. If and when a fuel particle's speed exceeds 12 units, it will be considered to be a combustion particle. At the time of ignition, the parameters \( v \) and \( V \) will be prescribed so that particles in the range \( 0 \leq x \leq 2.1 \) will be combustion particles while all others are fuel particles. A combustion particle will have its velocity increased by the factor \( C \) every \( T \) time steps until its speed exceeds 300, at which time its velocity will be reset to zero and it will be considered to be a burned particle.

Finally, we will allow symmetric particle reflection from the walls. However, the velocity of each reflected particle will be multiplied by the positive parameter \( d \). A choice \( d < 1 \) will imply transmission of heat to the walls.

We consider next examples for various choices of the parameters \( v, V, C, T, \) and \( d \).
Fig. 1. The initial particle configuration.

Fig. 2. The initial ignition area at the left end.
EXAMPLES

In each of the following examples, the simulation was carried out on a CRAY X-MP/24 through $t_{8000}$. Each example required only 274 seconds of CPU time.

Case 1. Consider the parameter choices $v=3$, $V=60$, $C=1.75$, $T=50$, $d=0.90$. Figures 3(a)–3(g) show the combustion particles at every 1000 time steps through $t_{8000}$, at which time there remains only one particle. Figure 3(h) shows the fuel particles at $t_{8000}$. One can say that the combustion was relatively efficient since only 10 fuel particles have escaped combustion. Figure 3(i) shows the burned particles at time $t_{8000}$. This configuration is typical of all the cases yet to be discussed.

Case 2. Consider this time the parameter choices $v=1$, $V=80$, $C=1.5$, $T=70$, $d=1.0$. All the parameters are different from Case 1. The motion is shown in Figures 4(a)–4(h). The number of combustion particles is greater at each time step than in Case 1, one factor being that the parameter C is greater in the present case. Figure 4(i) shows the remaining fuel particles at $t_{8000}$.

Case 3. The parameters this time are $v=1$, $V=80$, $C=1.75$, $T=70$, $d=0.9$. The combustion particles are shown in Figures 5(a)–5(f) through $t_{6000}$, after which there is burnout. Figure 5(g) shows the remaining fuel particles after the rapid and efficient combustion of this case. The existence of an isolated, centrally located combustion particle in Figure 5(a) is interesting and a related, but more complex, configuration will be discussed in Case 6.

Case 4. The parameters this time are $v=3$, $V=80$, $C=1.75$, $T=70$, $d=1.0$. The rate of combustion increases over that of Case 3 and is shown in Figures 6(a)–6(d) through $t_{4000}$, after which time there is burnout. Figure 6(e) shows the remaining fuel particles at $t_{5000}$.

Case 5. Figures 7(a)–7(b) show the most rapid combustion exhibited thus far and the fewest fuel particles remaining after burnout at time $t_{8000}$. The combustion in this case is relatively explosive, yet the parameters were the same as for Case 1 with the single exception $d=1.0$, indicating the significance of the material structure of the walls.
Case 6. The parameter choices in this case are the same as in Case 2, with the single exception $C=1.75$. However, the results are remarkably different. Figures 8(a)–8(d) show the combustion particles through $t_{4000}$, after which time there is burnout. Figure 8(e) shows the fuel particles which remain after burnout at $t_{5000}$. Figure 8(b), however, suggests that the combustion particles have divided into two disjoint areas. It may be that the rapid combustion rate induced by $T=30$ and the relatively large ignition velocity $V=80$ have induced a compression wave which energizes the right end of the tube, thereby generating a right combustion area which is distinct from the left one. Verification that combustion has occurred in two disjoint regions is seen in Figures 8(f) and 8(g) which show, respectively, the fuel particles and the burned particles at $t_{2000}$. The final combustion stage of this case occurs at the center of the tube rather than at the right end, as in previous cases.

Case 7. In this final case, the parameters are $v=1, V=60, C=1.75, T=30, d=0.9$. As seen in Figures 9(a)–9(h), the result is a relatively small combustion area at each time step through $t_{8000}$, after which burnout occurs. Figure 9(i) shows the fuel particle which remain at $t_{8000}$ and indicates the relative inefficiency of the parameter combination $v=1$ with $V=60$.

The totality of computer examples run consisted of all 48 possible cases with $v=1,3; V=60,80, C=1.5,1.75; T=30,50,70; \text{ and } d=0.9,1.0$. In general, Cases 1-7, above, were typical of the results.

REMARKS

Though the general ideas developed in Section 2 can be applied to combustion in solids, liquids, and gases, the examples in Section 3 were motivated by the wide interest in cylindrical combustion engines. Mathematically, the related vapor combustion is exceptionally difficult to model because it is of a turbulent nature and not usually accessible through continuum models. However, the turbulent character of the particle combustion in Figures 3–9 is readily apparent.

Finally, it may be noted that graphics in which the three types of particles, that is, fuel, combustion, and burned particles, are all shown at each time step, but in a different color, yield most impressive results.
(a) $t_{1000}$

(b) $t_{2000}$

(c) $t_{3000}$

(d) $t_{4000}$

(e) $t_{5000}$

(f) $t_{6000}$

(g) $t_{7000}$

(h) $t_{8000}$

(i) $t_{8000}$

(j) $t_{8000}$

Fig. 3. $v=3.0$, $v=60.0$, $c=1.75$, $T=50.0$, $d=0.9$. 
Fig. 4. $v=1.0$, $V=80.0$, $C=1.5$, $T=70.0$, $d=1.0$. 
Fig. 5. $v=1.0$, $V=80.0$, $C=1.75$, $T=70.0$, $d=0.9$. 
Fig. 6. \( v=3, \ V=80, \ C=1.75, \ T=70, \ d=1.0 \).
Fig. 7. $v=3.0$, $V=60.0$, $C=1.75$, $T=50.0$, $d=1.0$. 
Fig. 8. \( v=1.0, \ V=80.0, \ C=1.75, \ T=70.0, \ d=1.0. \)
Fig. 9. v=1.0, V=60.0, C=1.75, T=30, d=0.9.
ADDITIONAL REFERENCES