

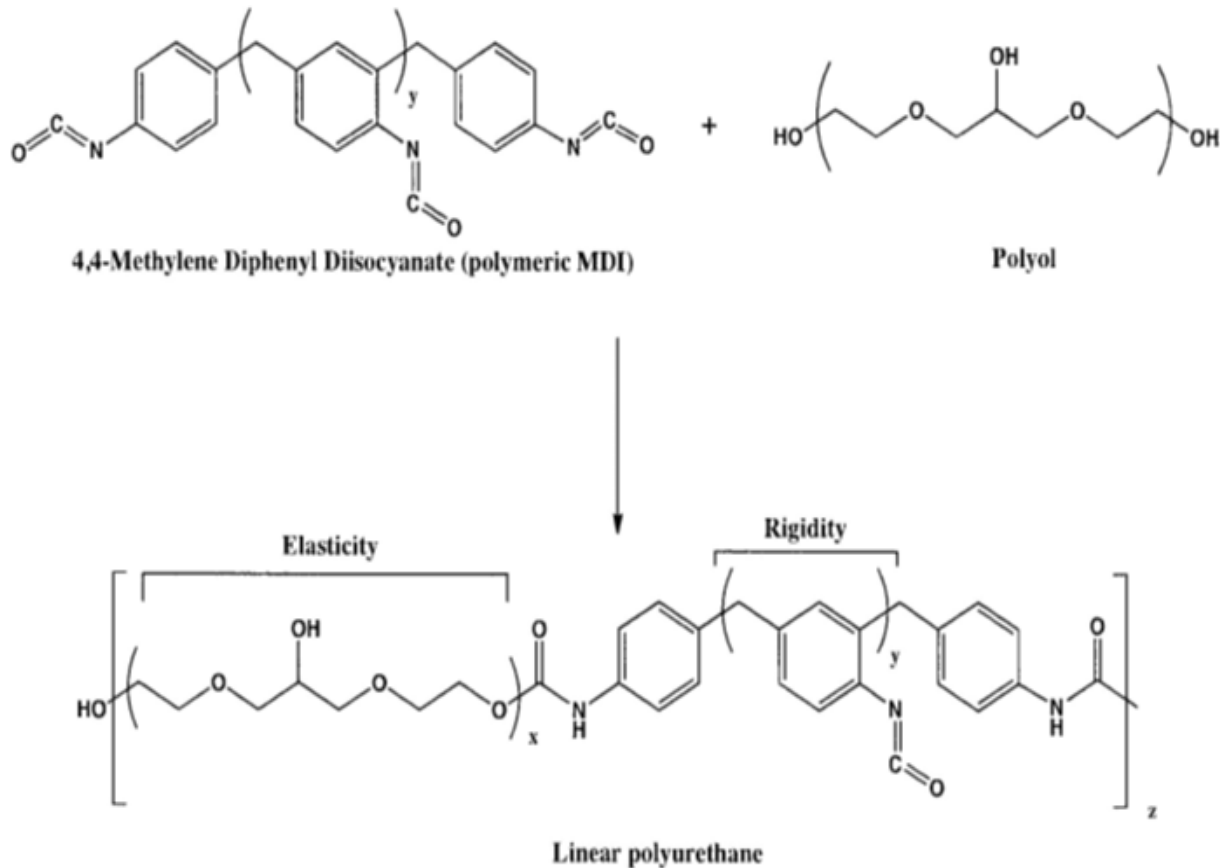
Diffusion Rates of Flame Retardants in Polyurethane Foam

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Polyurethane

- Product of step-growth polymerization between a monomer with at least two isocyanate functional groups and another monomer with at least two hydroxyl or alcohol groups in the presence of a catalyst
- Different monomers and additives determine physical properties of material
- Used in insulation foam, suspension bushings, adhesives, print rollers and many other applications



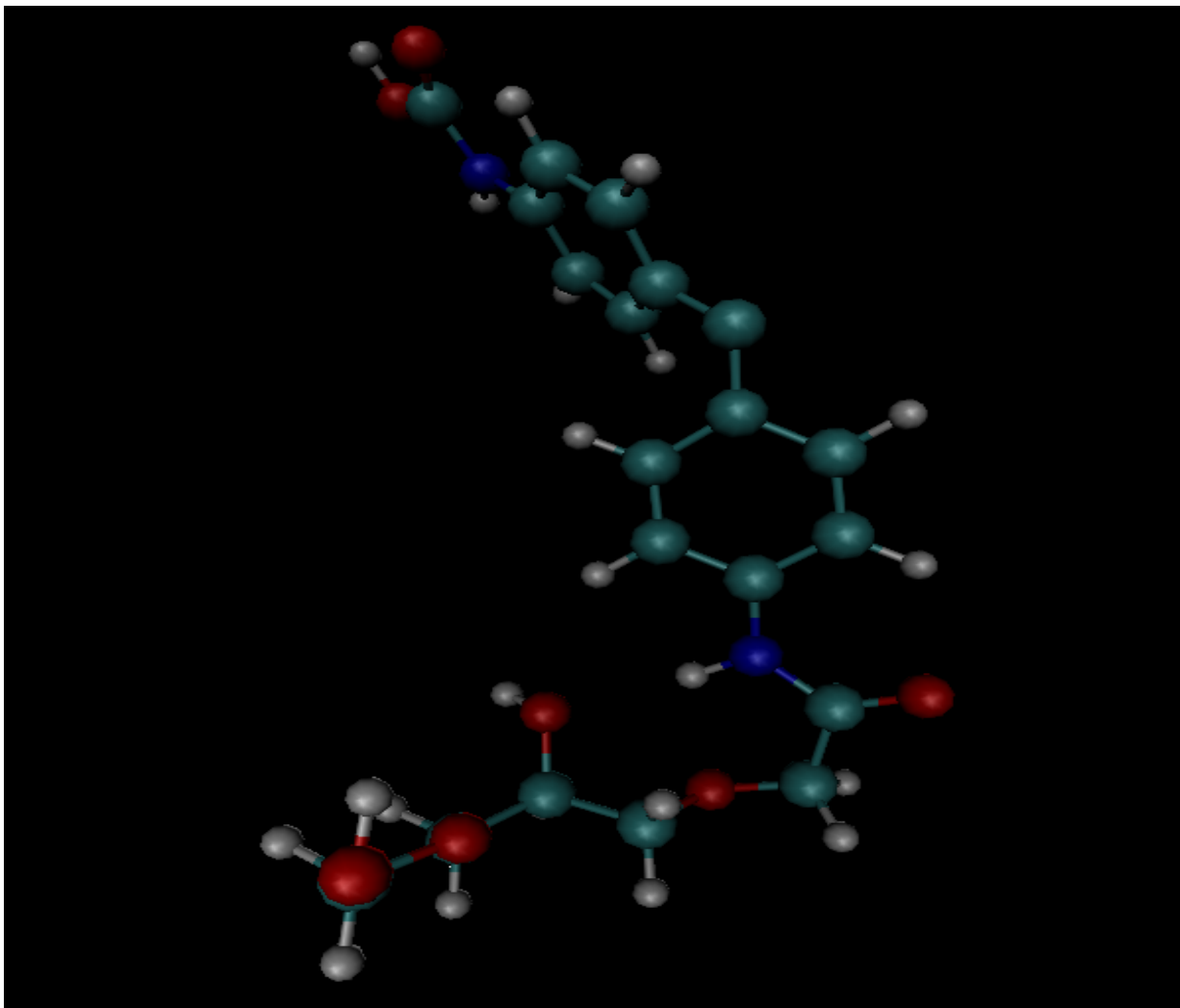
- Synthesized by reacting polymeric MDI with a polyol followed by crosslinking with butane diol to create a polyurethane thermoset
- Most commonly used in automotive seat cushioning and furniture

Research Goal

- Polyurethane is highly flammable in its raw state
- Production companies must introduce flame retardant molecules in the form of powders and liquids to make the polymer more stable
- Must know the best temperature and density of the materials for optimal diffusion of the flame retardant

Simulation Methods

- Polyurethane molecule and flame retardant molecules built in Molden
- Structures optimized on Louisiana Optical Network Initiative (LONI) supercomputers
- Script written for Large Atomic/Molecular Massively Parallel Simulator (LAMMPS) of single molecules
- Fortran code using Monte Carlo algorithm to replicate polyurethane molecule and generate environment for flame retardant diffusion tests
- LAMMPS output can then be visualized in VMD



Optimized polyurethane molecule

```
jparro@qb1:~/lammps/Polyurethane
#Polyurethane Input File
units          real
atom_style     molecular
bond_style     harmonic
pair_style     lj/cut 7.0
angle_style    harmonic
dihedral_style hybrid opls charmm

boundary p p p

read_data      data.poly

log            log.poly

velocity all create 375.0 97658764

group ***

fix           1          all nve

thermo_style  custom step etotal pe ke epair
thermo       ***
```

Input script for polyurethane molecule

```
jparro@qbl:~/lammps/Polyurethane
c   loop over molecules
    do k1=1,nmol
c   try to move com
      dx=delss*(unirand(ix)-0.5d0)
      dy=delss*(unirand(iy)-0.5d0)
      dz=delss*(unirand(iz)-0.5d0)
      call potcalc(k1,e0)
      do i1=1,natoms
        r(1,i1,k1)=r(1,i1,k1)+dx
        r(2,i1,k1)=r(2,i1,k1)+dy
        r(3,i1,k1)=r(3,i1,k1)+dz
      enddo
      call potcalc(k1,e1)
      trans=-(e1-e0)/temp
      rn=log(unirand(ia))
      if(trans .lt. log(unirand(ia))) then
        n1=n1+1
        do i1=1,natoms
          r(1,i1,k1)=r(1,i1,k1)-dx
          r(2,i1,k1)=r(2,i1,k1)-dy
          r(3,i1,k1)=r(3,i1,k1)-dz
        enddo
      endif
    enddo
  enddo
endif
```

242,1 59%

Monte Carlo code for creating environment


```
jparro@qbl:~/lammmps/Polyurethane
Reading data file ..
  orthogonal box = (-9.44326 -9.44326 -9.44326) to (9.44326 9.44326 9.44326)
  2 by 2 by 2 processor grid
  256 atoms
Setting up run ...
Memory usage per processor = 1.54811 Mbytes
Step Elapsed Temp Press PotEng KinEng TotEng
   0         0         0         1 0.037851562         0 1.4941406 1.49414
06
  100       100         0         1 0.037851562         0 1.4941406 1.49414
06
  200       200         0         1 0.037851562         0 1.4941406 1.49414
06
  300       300         0         1 0.037851562         0 1.4941406 1.49414
06
  400       400         0         1 0.037851562         0 1.4941406 1.49414
06
  500       500         0         1 0.037851562         0 1.4941406 1.49414
06
  600       600         0         1 0.037851562         0 1.4941406 1.49414
06
  700       700         0         1 0.037851562         0 1.4941406 1.49414
06
                                     26,21                                     15%
```

Output file for simulation

Acknowledgements

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- Dr. Randall Hall, Chemistry Dept., LSU
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- Large Atomic/Molecular Massively Parallel Simulator (LAMMPS)
- Humphrey, W., Dalke, A. and Schulten, K., "VMD - Visual Molecular Dynamics", J. Molec. Graphics, 1996, vol. 14, pp. 33-38. (VMD)
- G.Schaftenaar and J.H. Noordik, "Molden: a pre- and post-processing program for molecular and electronic structures", J. Comput.-Aided Mol. Design, 14 (2000) 123-134 (Molden)