```
units       nano
variable    T_wall  equal   120
variable    T_fluid equal   200
variable    spring_constant    equal    70.0e3

dimension    2
boundary    p    f    p
atom_style    atomic
neighbor    3.0    bin
neigh_modify    delay    1    check    yes

#-----------------------model---------------------------
lattice       sq        0.4
region        box        block    0    200    0    60    -0.25    0.25
create_box    2    box

#-----------------------region---------------------------
region         r_bot_wall   block   INF INF INF    2    INF INF
region         r_top_wall   block   INF INF  57.0   INF   INF INF

region         r_bot_wall_1 block   INF INF INF     0.2 INF INF
region         r_bot_wall_2 block   INF INF 0.2     1.2 INF INF
region         r_bot_wall_3 block   INF INF 1.2     2.1 INF INF

region         r_top_wall_1   block   INF INF  57.0   57.1   INF INF
region         r_top_wall_2   block   INF INF  57.9   58.1   INF INF
region         r_top_wall_3   block   INF INF  58.9   59.1   INF INF



region         r_flow       block   INF INF 2.01   56.99   INF INF
region         r_flow_1     block   INF INF 5.01   53.99   INF INF
region         r_flow_f     block   0   3   2.00   57.00   INF INF
region         r_flow_t     block   3   7   2.00   57.00   INF INF  #先定义，以后再用
region         r_flow_o     block   7   INF   2.00   57.00   INF INF

#-------------------------create atoms----------------------
create_atoms    1   region      box
delete_atoms        region      r_flow

group           g_bot_wall      region  r_bot_wall
group           g_top_wall      region  r_top_wall
group           g_boundary      union   g_bot_wall  g_top_wall


create_atoms    2   random      10000   987654   r_flow_1

group           g_flow          type     2

group           g_dynamic_f     dynamic     g_flow  region  r_flow_f    every   1
group           g_dynamic_t     dynamic     g_flow  region  r_flow_t    every   1
group           g_dynamic_o     dynamic     g_flow  region  r_flow_o    every   1

mass            1     0.0001793448        #179.3448/1.0e6   #氩银参数
mass            2     0.000066424         #66.424/1.0e6

#---------------------------LJ potential-----------------
pair_style    lj/cut    0.85125                           #氩银参数
pair_coeff    1   1     83.5    0.2475    0.85125
```

```
pair_coeff    2   2     1.657    0.3405    0.85125
pair_coeff    1   2    0.9613    0.2978    0.85125


#------------------------initialization velocity------------
velocity     g_boundary           create    ${T_wall}    987654    dist    gaussian
velocity     g_flow               create    ${T_wall}    987654    dist    gaussian

#------------------------spring model for wall atoms-----------------------------------------------
fix            spring_boundary_wall            g_boundary        spring/self
${spring_constant}


#------------------------energy minimization-------------------------------------
minimize    1.0e-6    1.0e-9    10000     20000
min_style    cg

#------------------------thermostat for boundary---------------------------------
compute        th_com_wall      g_bot_wall    temp
fix            th_fix_wall      g_bot_wall    temp/rescale    1   ${T_wall}    ${T_wall}    0.1    1
fix_modify     th_fix_wall      temp          th_com_wall

compute        th_com_wall_0      g_top_wall    temp
fix            th_fix_wall_0      g_top_wall    temp/rescale    1   ${T_wall}    ${T_wall}    0.1
1
fix_modify     th_fix_wall_0      temp          th_com_wall_0

#------------------------thermostat for liquid-----------------------------------
compute          th_com_flow     g_flow        temp
#fix             th_scale_flow   g_flow        nvt    temp     ${T_fluid}    ${T_fluid}    1.0e-3
fix              th_scale_flow   g_flow   temp/rescale    1   ${T_wall}    ${T_wall}    0.1    1
fix_modify       th_scale_flow   temp          th_com_flow
fix            1   g_flow   nve

fix             2D              all     enforce2d

fix            spring_recenter_1                g_boundary        recenter       INIT    INIT
INIT

#----------------------------------equilibrium-----------------------------------------
compute     ps_com_sample_20       g_flow    temp

dump         5a      g_flow       custom     500000    dump.quan.* id     type     x   y   vx  vy
thermo    10000
timestep     0.00001
run          200000

#----------------------------------fluid definition-------------------------------
unfix            th_scale_flow
unfix            1
unfix            spring_recenter_1

fix              flow_definition        g_dynamic_f      addforce    2.0    0.0    0.0

#velocity       g_flow       set     5000.0  NULL   NULL    sum    yes    units    box

#添加Langevin等温
#compute     rs_tank_right_kuai       g_flow       chunk/atom  bin/1d    y   0.8   4.4      units
box
```

```
#compute     rs_temp_right_kuai       g_flow       temp/chunk    rs_tank_right_kuai     temp    com
yes
#fix         rs_scale_right           g_flow       langevin    ${T_fluid}    ${T_fluid}  1.0e-3
699483
#fix_modify  rs_scale_right           temp                rs_temp_right_kuai

compute     fd_com       g_flow      temp/profile   1   0   0   xy  1   1
fix         fd_temp      g_flow      langevin    ${T_fluid}    ${T_fluid}  0.001  699483
fix_modify  fd_temp       temp        fd_com


fix            fd_time_1             g_flow     nve

fix            spring_recenter_2                g_boundary        recenter       INIT    INIT
INIT

#检测质心速度
run        0
variable    flow_vcm_xa    equal       vcm(g_flow,x)
variable    flow_vcm_ya    equal       vcm(g_flow,y)

variable    flow_vcm_xo    equal       vcm(g_dynamic_o,x)
variable    flow_vcm_yo    equal       vcm(g_dynamic_o,y)

thermo     10000
thermo_style custom step temp pe etotal press   v_flow_vcm_xa   v_flow_vcm_ya    v_flow_vcm_xo
v_flow_vcm_yo

compute          wall_t  g_boundary   temp
thermo_modify    temp  wall_t

timestep     0.00001
run          300000

#----------------------------------去整体温度控制，转而控制局部温度----------------------
unfix       fd_temp
unfix       fd_time_1
unfix       spring_recenter_2

compute             rd_com        g_dynamic_t      temp/profile   1   0   0   xy  1   1
compute_modify      rd_com        dynamic/dof      yes
fix                 rd_temp       g_dynamic_t      langevin    ${T_fluid}    ${T_fluid}  0.001
699483
fix_modify          rd_temp       temp             rd_com

fix            fd_time_2             g_flow     nve

fix            spring_recenter_3     g_boundary        recenter       INIT    INIT    INIT

thermo_modify    temp  rd_com
timestep     0.00001
run          1000000

#----------------------------------sampling---------------------------------------


#----------------------- xy方向采样----------------------------
```

```
#10*10块
compute             2ps_com_20_1       g_flow    chunk/atom  bin/2d  x   2.8     7.72     y   0.8
2.2    bound    x   2.8 80.0  bound    y  0.8   22.8  units box
compute             10nps_com_0        g_dynamic_o      temp/profile   1   0   0    y   10
compute_modify      10nps_com_0        dynamic/dof      yes
fix                 10nps_re_0         all    ave/chunk    2     1000000     3600000    2ps_com_20_1
vx   vy       density/number    temp     bias      10nps_com_0    file    nn_10_1.out    format
%20.16g



#---------------------------------result-----------------------------------

thermo      50000

timestep    0.00001
run         3800000
```