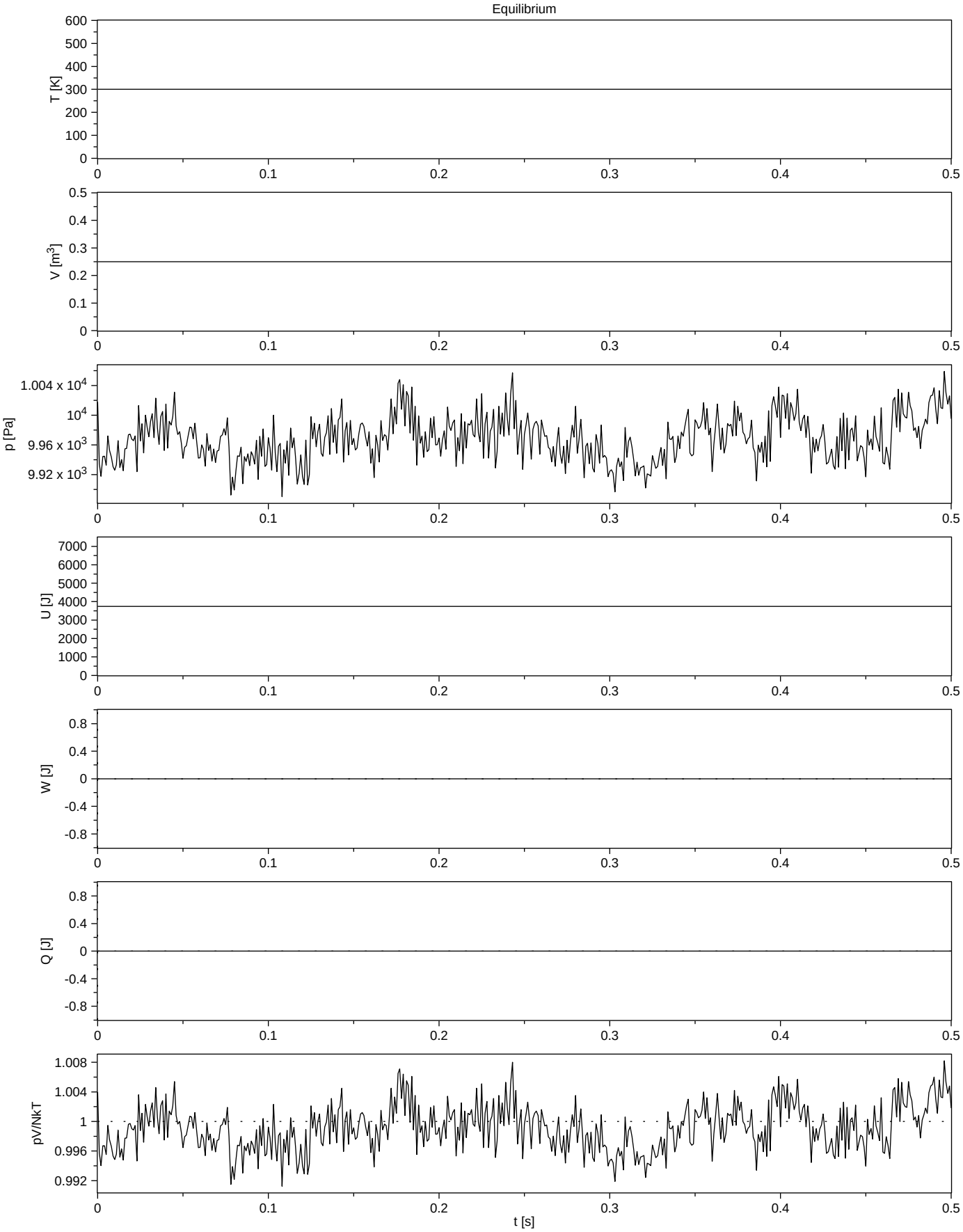
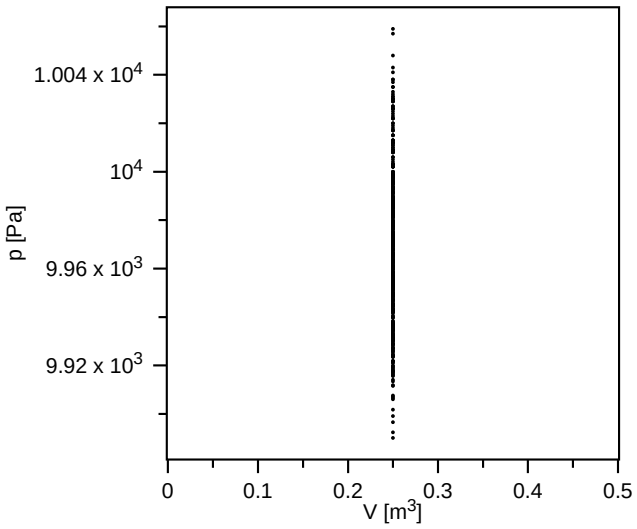
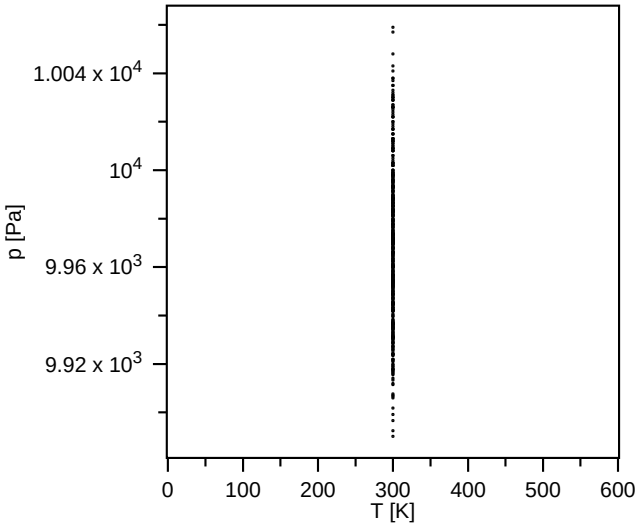
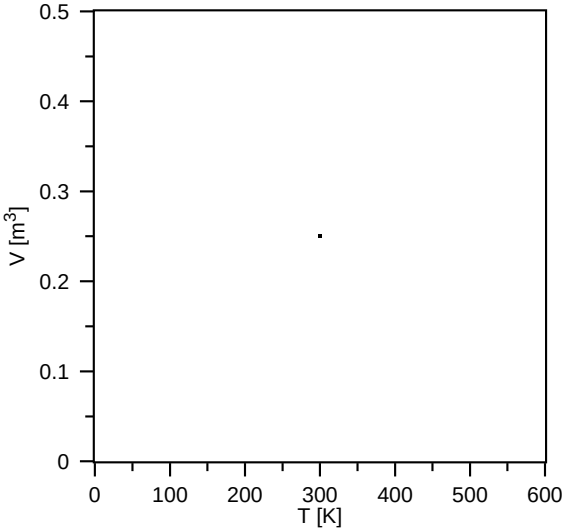
Simulation at constant energy and volume



Simulation at constant energy and volume





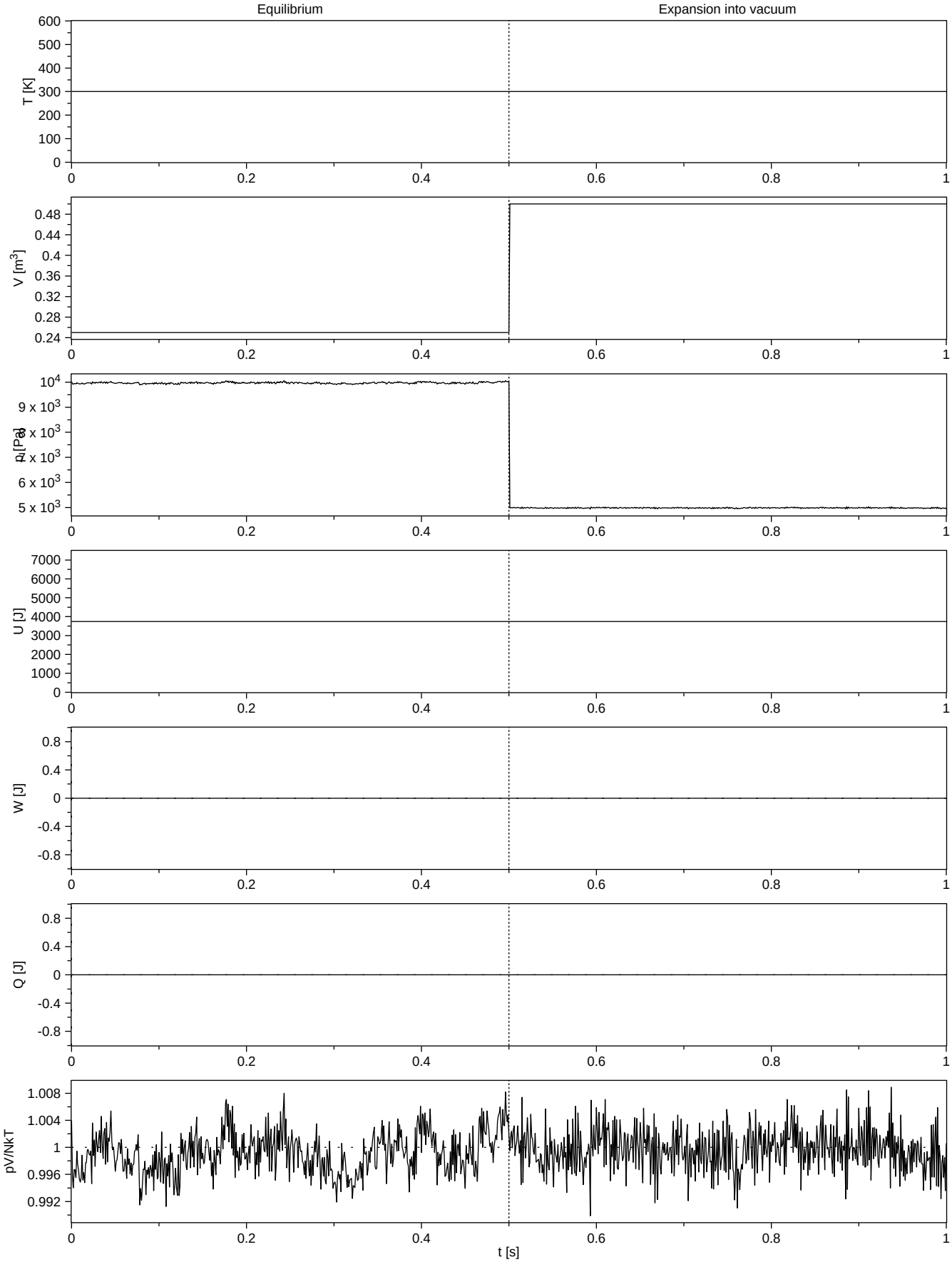


Input file ex1-fixed.txt:

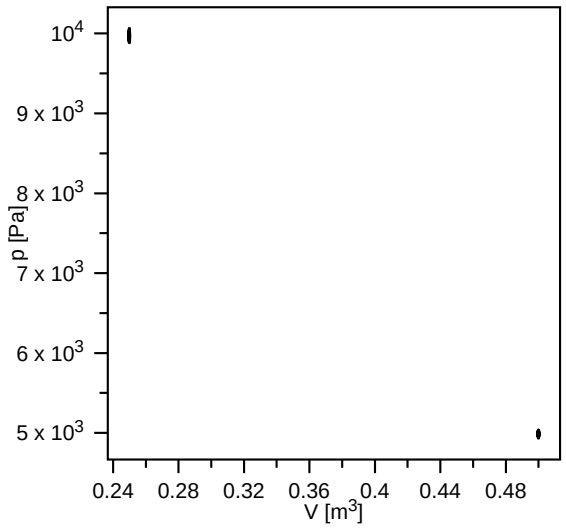
```
title='Simulation at constant energy and volume'

# ------ initial parameter values ------

ntotal=6.02214E23         # total number of particles (1 mol)
n=50000                   # number of simulated particles
mass=4.64951E-26          # mass of particles [kg] (N2 molecule)
box=1.0,1.0,0.25          # initial box size [m]
tempinit=300.0            # initial temperature [K]
seed=3771                 # random number generator seed
dt=2.0E-5                 # time step [s]
wallmass=0                # boxer: mass of movable wall [kg] (0 for rigid wall)
rheat=1000.0              # heater: heating events per particle and unit time [1/s]
rmix=100.0                # mixer: mixing events per particle and unit time [1/s]
dtprint=0.001             # time interval for reporting [s]
dtave=0.001               # time interval for averaging [s]
report='Time,Step,Temperature,Volume,Pressure,ExtPressure,Energy,Work,Heat,Ideality'
                          # quantities to report
#plotfile='start*.grf'     # plot file (* will be replaced by an incrementing counter)

# ------ stage-specific parameter values ------

stage='Equilibrium'
  duration=0.5            # duration [s]
  tempheater=0.0          # heat bath temperature [K] (0 for adiabatic)
  wallmass=0.0            # mass of movable wall [kg] (0 for rigid wall)
  pressext0=9977.4        # external pressure at start of stage [Pa]
  pressext=9977.4         # external pressure at end of stage [Pa]
```

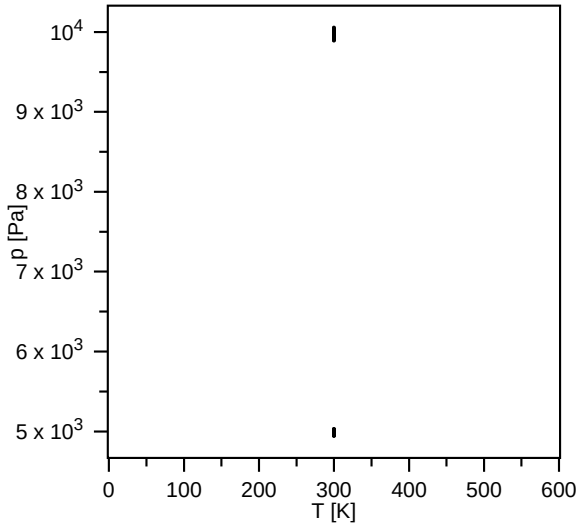
```
Energy-Energy0-Heat+Work     : -9.0949E-13 J
Total work done by system    :           0 J
Total heat brought to system :           0 J
Total entropy change         :           0 J/K
```

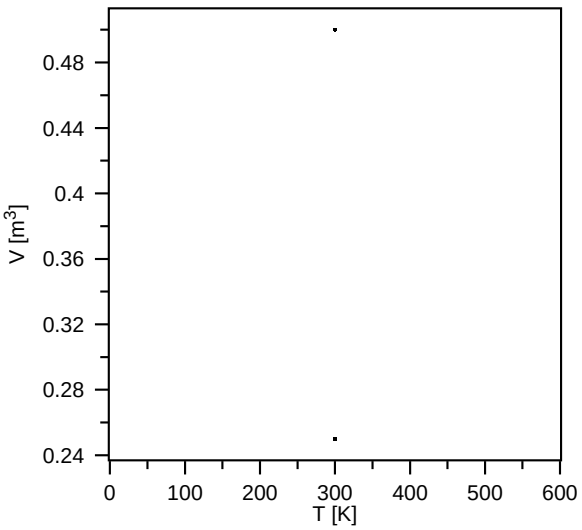
Expansion into vacuum



Expansion into vacuum





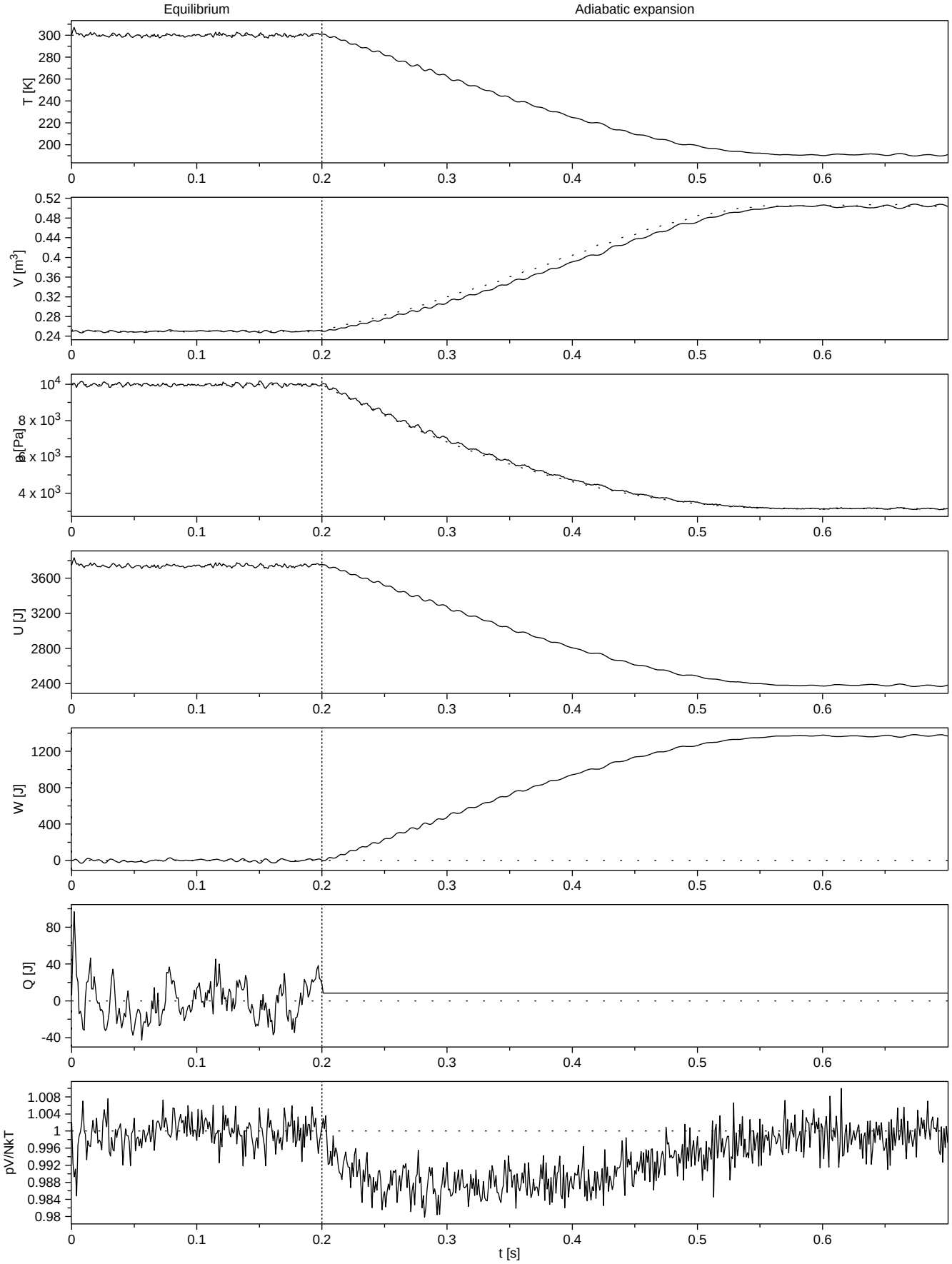


Input file ex2-vacuum.txt:

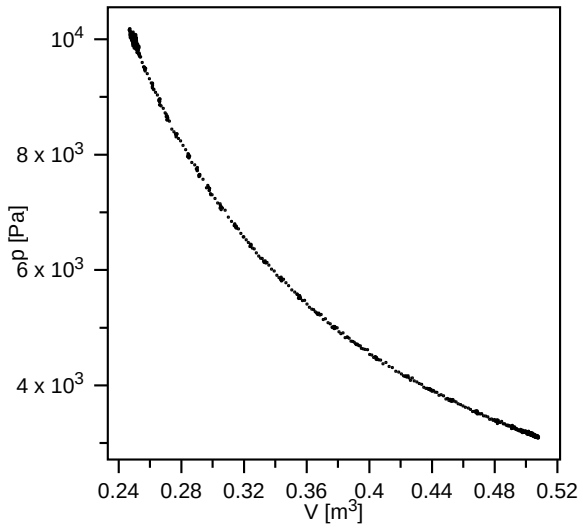
```
title='Expansion into vacuum'

# ------ initial parameter values ------

ntotal=6.02214E23         # total number of particles (1 mol)
n=50000                   # number of simulated particles
mass=4.64951E-26          # mass of particles [kg] (N2 molecule)
box=1.0,1.0,0.25          # initial box size [m]
tempinit=300.0            # initial temperature [K]
seed=3771                 # random number generator seed
dt=2.0E-5                 # time step [s]
wallmass=0                # boxer: mass of movable wall [kg] (0 for rigid wall)
rheat=1000.0              # heater: heating events per particle and unit time [1/s]
rmix=100.0                # mixer: mixing events per particle and unit time [1/s]
dtprint=0.001             # time interval for reporting [s]
dtave=0.001               # time interval for averaging [s]
report='Time,Step,Temperature,Volume,Pressure,ExtPressure,Energy,Work,Heat,Ideality'
                          # quantities to report
#plotfile='start*.grf'     # plot file (* will be replaced by an incrementing counter)

# ------ stage-specific parameter values ------

stage='Equilibrium'
  duration=0.5            # duration [s]
  tempheater=0.0          # heat bath temperature [K] (0 for adiabatic)
  wallmass=0.0            # mass of movable wall [kg] (0 for rigid wall)
  pressext0=9977.4        # external pressure at start of stage [Pa]
  pressext=9977.4         # external pressure at end of stage [Pa]

stage='Expansion into vacuum'
  box=1.0,1.0,0.5         # initial box size [m]
```

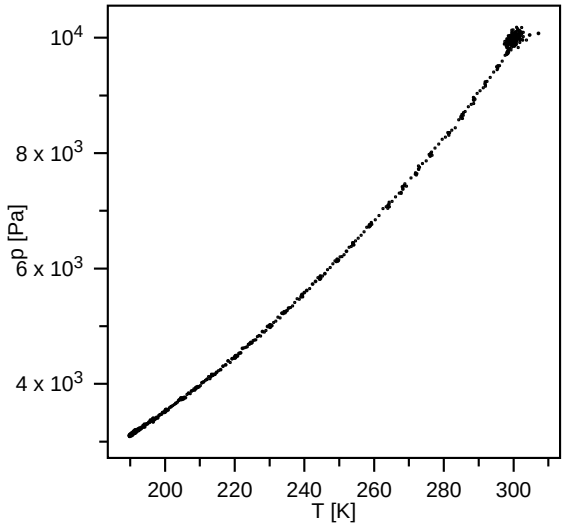
```
Energy-Energy0-Heat+Work     :  -3.638E-12 J
Total work done by system    :           0 J
Total heat brought to system :           0 J
Total entropy change         :           0 J/K
```

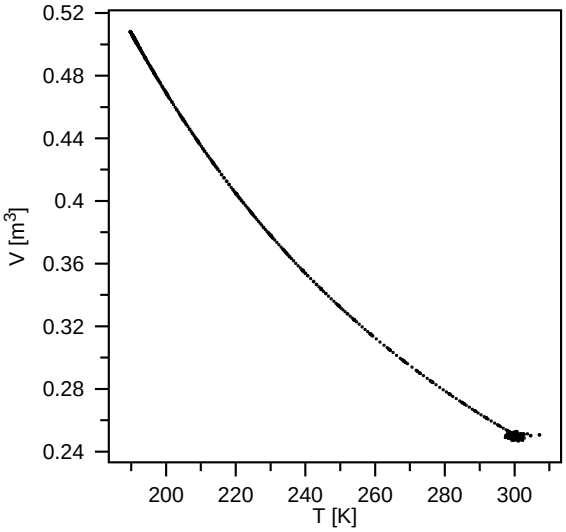
Adiabatic expansion



Adiabatic expansion





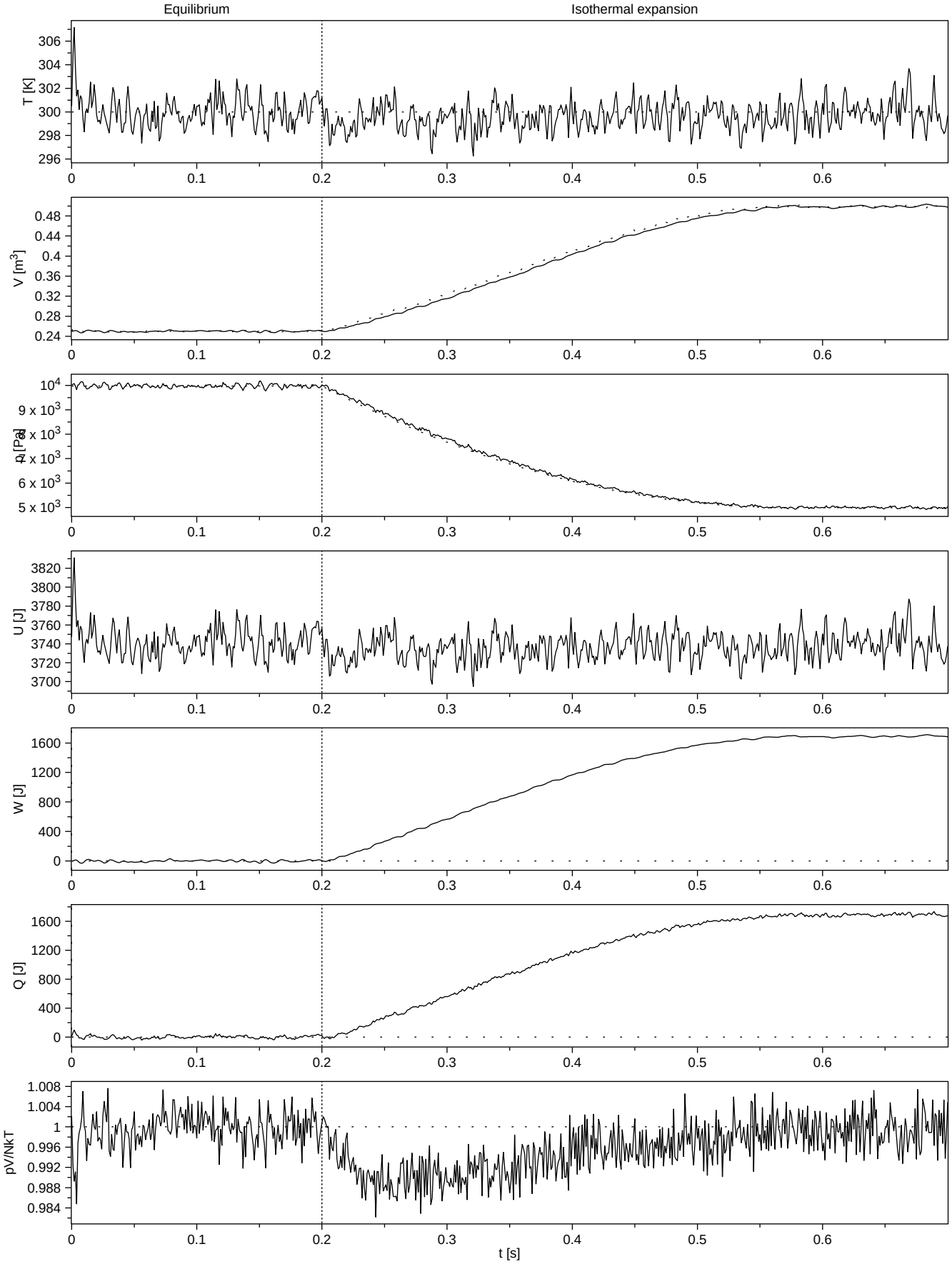


Input file ex3-adiabatic.txt:

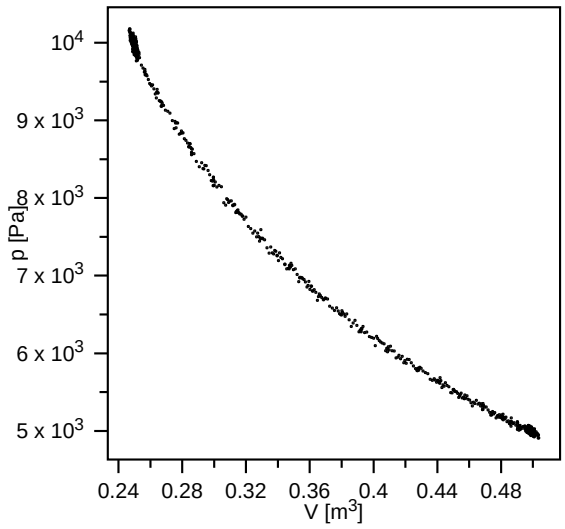
```
title='Adiabatic expansion'

# ------ initial parameter values ------

ntotal=6.02214E23         # total number of particles (1 mol)
n=50000                   # number of simulated particles
mass=4.64951E-26          # mass of particles [kg] (N2 molecule)
box=1.0,1.0,0.25          # initial box size [m]
tempinit=300.0            # initial temperature [K]
seed=3771                 # random number generator seed
dt=2.0E-5                 # time step [s]
wallmass=0                # boxer: mass of movable wall [kg] (0 for rigid wall)
rheat=1000.0              # heater: heating events per particle and unit time [1/s]
rmix=100.0                # mixer: mixing events per particle and unit time [1/s]
dtprint=0.001             # time interval for reporting [s]
dtave=0.001               # time interval for averaging [s]
report='Time,Step,Temperature,Volume,Pressure,ExtPressure,Energy,Work,Heat,Ideality'
                          # quantities to report
#plotfile='start*.grf'     # plot file (* will be replaced by an incrementing counter)

# ------ stage-specific parameter values ------

stage='Equilibrium'
  duration=0.2            # duration [s]
  tempheater=300.0        # heat bath temperature [K] (0 for adiabatic)
  wallmass=0.2            # mass of movable wall [kg] (0 for rigid wall)
  pressext0=9977.4        # external pressure at start of stage [Pa]
  pressext=9977.4         # external pressure at end of stage [Pa]

stage='Adiabatic expansion'
  duration=0.5            # duration [s]
  tempheater=0.0          # heat bath temperature [K] (0 for adiabatic)
  pressext=3142.7         # external pressure at end of stage [Pa]
```

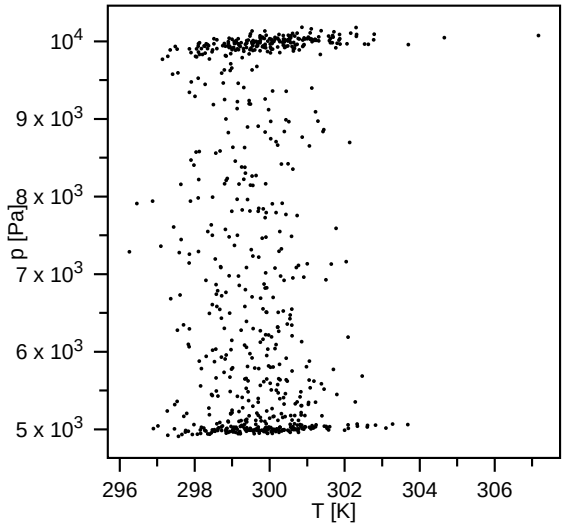
```
Energy-Energy0-Heat+Work     :  -9.959E-11 J
Total work done by system    :      1365.7 J
Total heat brought to system :      8.3095 J
Total entropy change         :   -0.021761 J/K
```

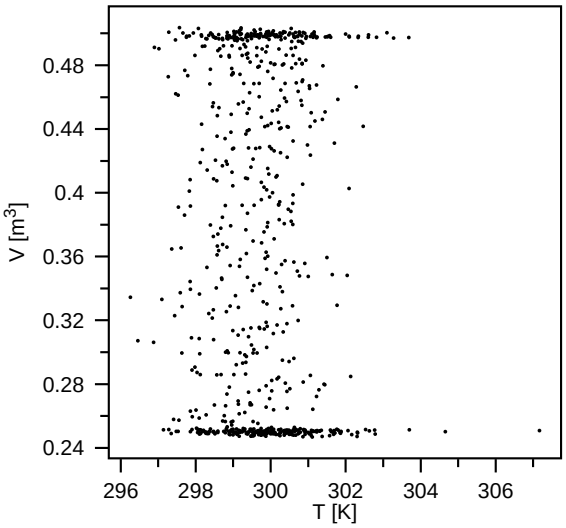
Isothermal expansion



Isothermal expansion





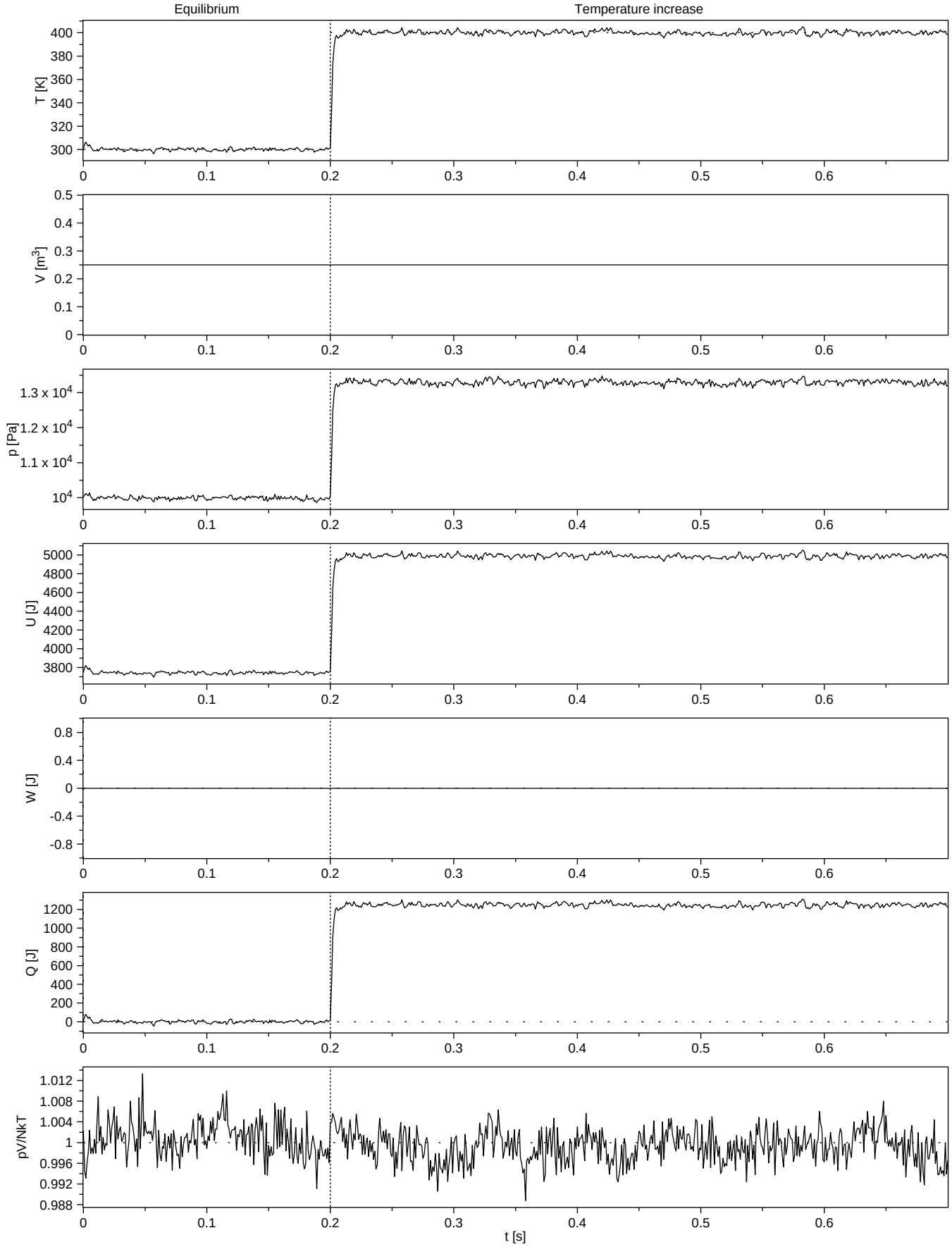


Input file ex4-isothermal.txt:

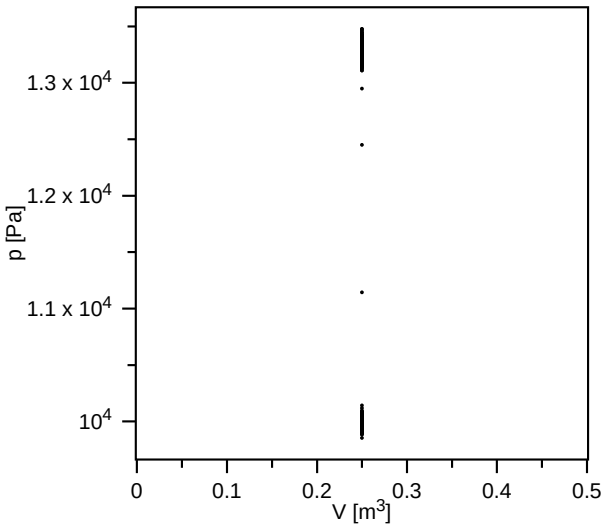
```
title='Isothermal expansion'

# ------ initial parameter values ------

ntotal=6.02214E23         # total number of particles (1 mol)
n=50000                   # number of simulated particles
mass=4.64951E-26          # mass of particles [kg] (N2 molecule)
box=1.0,1.0,0.25          # initial box size [m]
tempinit=300.0            # initial temperature [K]
seed=3771                 # random number generator seed
dt=2.0E-5                 # time step [s]
wallmass=0                # boxer: mass of movable wall [kg] (0 for rigid wall)
rheat=1000.0              # heater: heating events per particle and unit time [1/s]
rmix=100.0                # mixer: mixing events per particle and unit time [1/s]
dtprint=0.001             # time interval for reporting [s]
dtave=0.001               # time interval for averaging [s]
report='Time,Step,Temperature,Volume,Pressure,ExtPressure,Energy,Work,Heat,Ideality'
                          # quantities to report
#plotfile='start*.grf'     # plot file (* will be replaced by an incrementing counter)

# ------ stage-specific parameter values ------

stage='Equilibrium'
  duration=0.2            # duration [s]
  tempheater=300.0        # heat bath temperature [K] (0 for adiabatic)
  wallmass=0.2            # mass of movable wall [kg] (0 for rigid wall)
  pressext0=9977.4        # external pressure at start of stage [Pa]
  pressext=9977.4         # external pressure at end of stage [Pa]

stage='Isothermal expansion'
  duration=0.5            # duration [s]
  pressext=4988.7         # external pressure at end of stage [Pa]
```

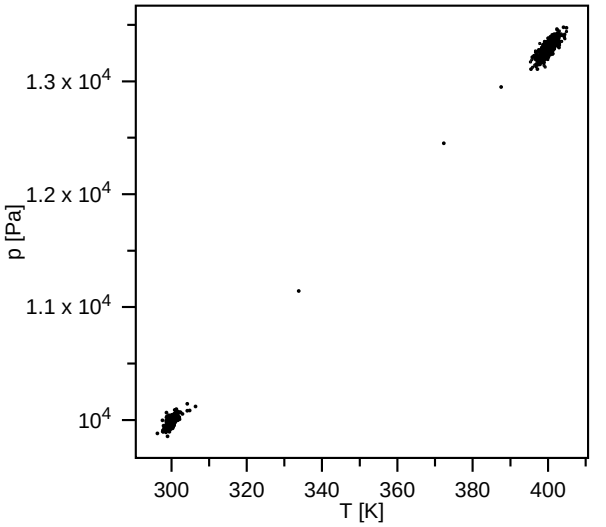
```
Energy-Energy0-Heat+Work     : -1.1005E-10 J
Total work done by system    :      1681.7 J
Total heat brought to system :      1680.4 J
Total entropy change         :      5.4396 J/K
```

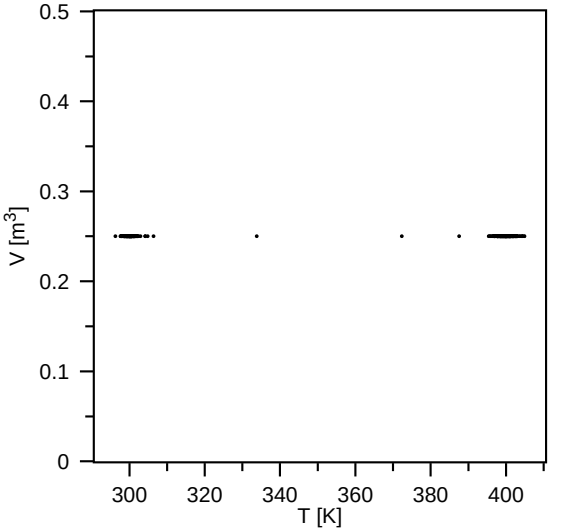
Heat capacity at constant volume



Heat capacity at constant volume





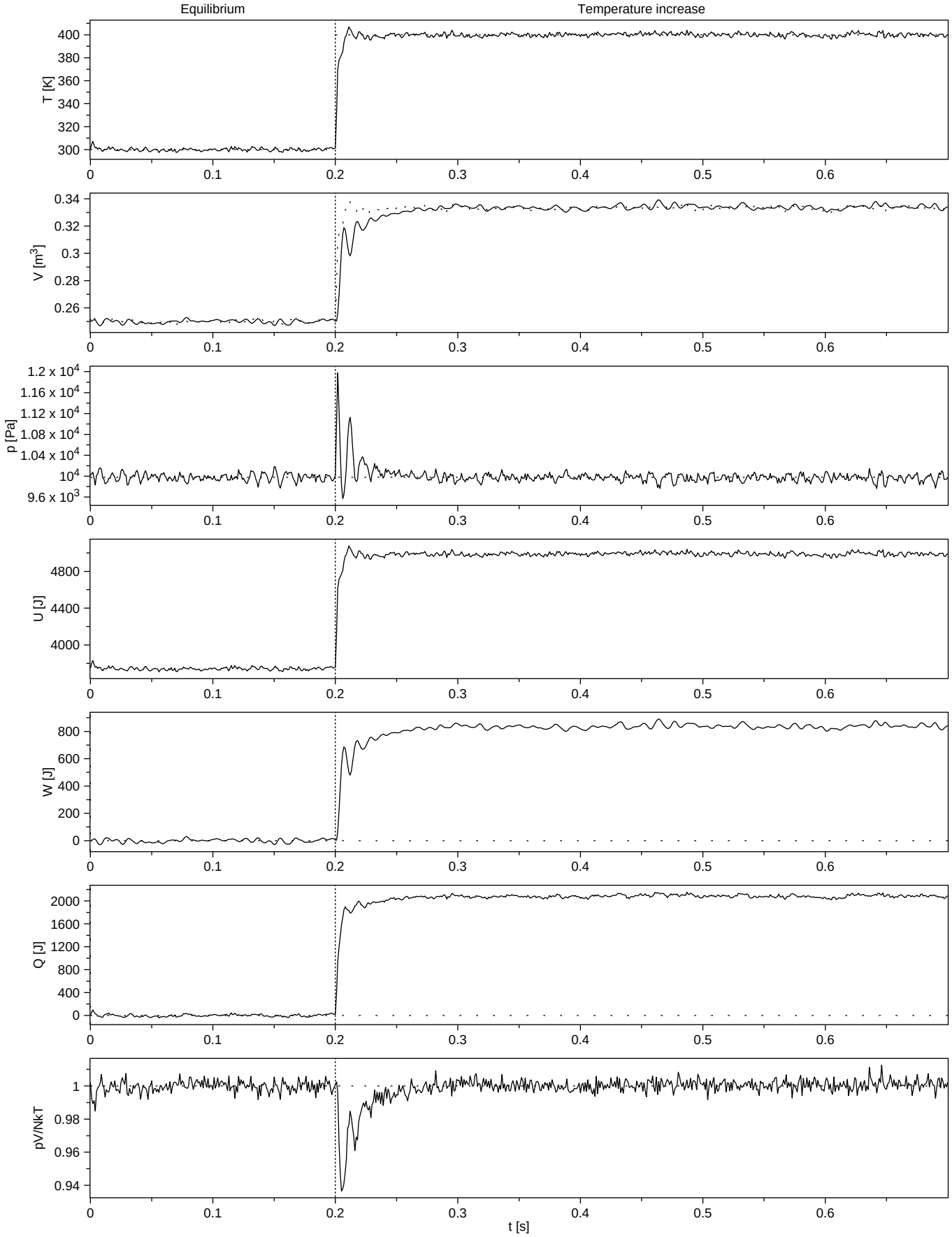



```
Energy-Energy0-Heat+Work     :  9.0949E-13 J
Total work done by system    :           0 J
Total heat brought to system :      1226.5 J
Total entropy change         :      3.3558 J/K
```

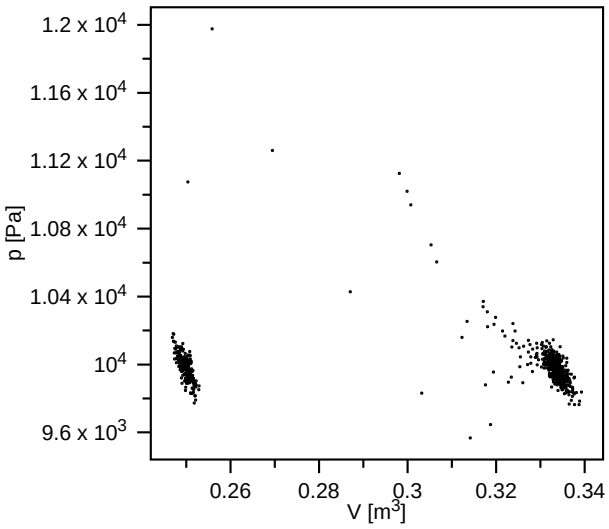
Input file ex5-Cv.txt:

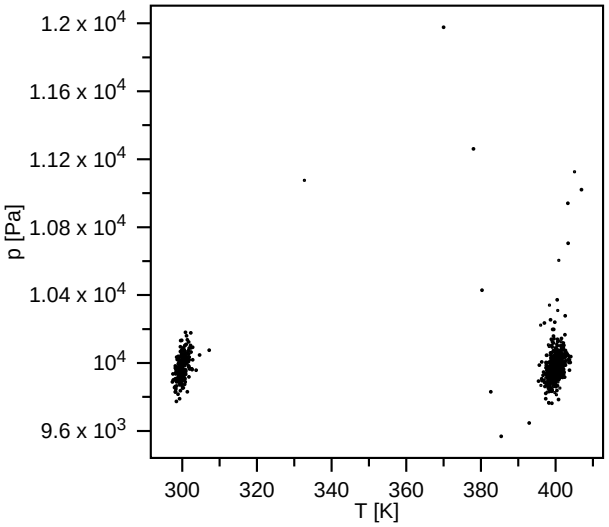
```
title='Heat capacity at constant volume'

# ------ initial parameter values ------

ntotal=6.02214E23         # total number of particles (1 mol)
n=50000                   # number of simulated particles
mass=4.64951E-26          # mass of particles [kg] (N2 molecule)
box=1.0,1.0,0.25          # initial box size [m]
tempinit=300.0            # initial temperature [K]
seed=3771                 # random number generator seed
dt=2.0E-5                 # time step [s]
wallmass=0                # boxer: mass of movable wall [kg] (0 for rigid wall)
rheat=1000.0              # heater: heating events per particle and unit time [1/s]
rmix=100.0                # mixer: mixing events per particle and unit time [1/s]
dtprint=0.001             # time interval for reporting [s]
dtave=0.001               # time interval for averaging [s]
report='Time,Step,Temperature,Volume,Pressure,ExtPressure,Energy,Work,Heat,Ideality'
                          # quantities to report
#plotfile='start*.grf'     # plot file (* will be replaced by an incrementing counter)

# ------ stage-specific parameter values ------

stage='Equilibrium'
  duration=0.2            # duration [s]
  tempheater=300.0        # heat bath temperature [K] (0 for adiabatic)
  wallmass=0.0            # mass of movable wall [kg] (0 for rigid wall)

stage='Temperature increase'
  duration=0.5            # duration [s]
  tempheater=400.0        # heat bath temperature [K] (0 for adiabatic)
```

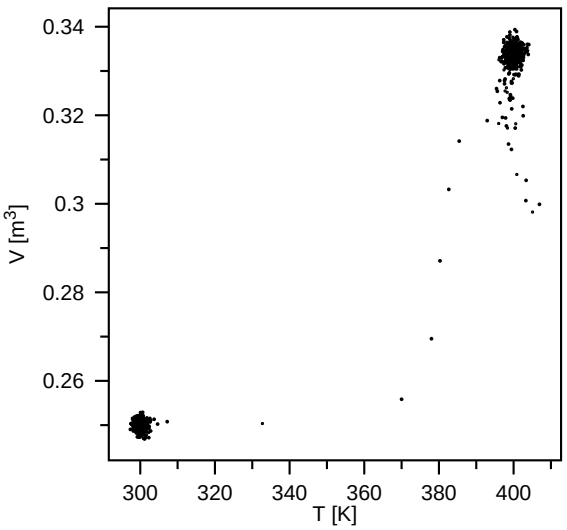
Heat capacity at constant pressure



Heat capacity at constant pressure








```
Energy-Energy0-Heat+Work     : -3.7653E-10 J
Total work done by system    :      840.63 J
Total heat brought to system :      2101.5 J
Total entropy change         :      5.6476 J/K
```

Input file ex5-Cp.txt:

```
title='Heat capacity at constant pressure'

# ------ initial parameter values ------

ntotal=6.02214E23         # total number of particles (1 mol)
n=50000                   # number of simulated particles
mass=4.64951E-26          # mass of particles [kg] (N2 molecule)
box=1.0,1.0,0.25          # initial box size [m]
tempinit=300.0            # initial temperature [K]
seed=3771                 # random number generator seed
dt=2.0E-5                 # time step [s]
wallmass=0                # boxer: mass of movable wall [kg] (0 for rigid wall)
rheat=1000.0              # heater: heating events per particle and unit time [1/s]
rmix=100.0                # mixer: mixing events per particle and unit time [1/s]
dtprint=0.001             # time interval for reporting [s]
dtave=0.001               # time interval for averaging [s]
report='Time,Step,Temperature,Volume,Pressure,ExtPressure,Energy,Work,Heat,Ideality'
                          # quantities to report
#plotfile='start*.grf'     # plot file (* will be replaced by an incrementing counter)

# ------ stage-specific parameter values ------

stage='Equilibrium'
  duration=0.2            # duration [s]
  tempheater=300.0        # heat bath temperature [K] (0 for adiabatic)
  wallmass=0.2            # mass of movable wall [kg] (0 for rigid wall)
  pressext0=9977.4        # external pressure at start of stage [Pa]
  pressext=9977.4         # external pressure at end of stage [Pa]

stage='Temperature increase'
  duration=0.5            # duration [s]
  tempheater=400.0        # heat bath temperature [K] (0 for adiabatic)
```