b) Temperatures
c) Com velocities
d) Volume forces

Figure 41  Comparison of the summarised local observables in several heterophasic nonequilibrium interfacial systems with strict and loose thermostats

N-Ar1Ar2-0.6-1.0-3346-3524-4.74x8.00x9.40-100-140-r1 and N-Ar1Ar2-0.6-1.0-3346-3524-4.74x8.00x9.40-100-140-loose; We include also their corresponding systems in the comparison.
b) Temperatures
c) Com velocities
d) Volume forces

e) Particle forces

f) Normal stresses

Figure 42  Comparison of the summarised local observables in the first homo- and heterophasic nonequilibrium interfacial systems N-Ar1Ar2-0.6-1.0-3346-3524-4.74x8.00x9.40-100-140 and N-Ar5Ar5-0.6-1.0-3346-3524-4.74x8.00x9.40-100-140; We include also their corresponding systems in the comparison.
Figure 43  Comparison of the mutual solubilities in the Ar1Ar2 and in the Ar5Ar5 mixture as function of the temperature

a) Velocities
b) Velocity components
c) Intensity

Figure 44  Comparison of the thermocapillary convection in Ar5Ar5 systems with different $z$-dimensions
a) Velocities
Figure 45  Comparison of the thermocapillary convection in Ar5Ar5 systems with different $y$-dimensions
Figure 46  Comparison of the thermocapillary convection in Ar5Ar5 systems with different y- and z-dimensions
Figure 47 Comparison of the local com velocities in Ar5Ar5 nonequilibrium interfacial systems that differ only in the temperature difference between the thermostated regions

Figure 48 Section of the Ar5Ar5 pxT-diagram at $x_{Ar5}=0.5$ with indication of the global pressures and temperatures in selected systems
a) Velocities
Int TCAvT.png

Int TCPres.png

b) Intensity

Figure 49  Comparison of the thermocapillary convection in several Ar5Ar5 systems that differ in the global temperatures and pressures
a) Velocities

b) Intensity

Figure 50  Comparison of the thermocapillary convection in several Ar5Ar5 systems that differ only in the values of the mixing parameter $\zeta$.

Figure 51  Cut of the Ar5Ar5 pxT diagram at $x_{Ar} \approx 0.5$ with indication of the global pressures and temperatures in the systems with different mixing parameter values $\zeta$. 
Figure 52 Comparison of the thermocapillary convection in Ar5Ar5 systems with different particle masses, $m_{ArA}$ and $m_{ArB}$

Figure 53 Cut of the Ar5Ar5 pX diagram at $x_{Ar} = 0.5$ with indication of the global pressures and temperatures in the systems with different particle masses, $m_{ArA}$ and $m_{ArB}$
a) Typical density \( z \)-dependence; We use the first homophasic nonequilibrium interfacial system as an example, N-Ar5Ar5-0.6-1.0-3346-3524-4.74x8.00x9.40-100-140.

b) Typical density \( y \)-dependence; We use the first homophasic nonequilibrium interfacial system as an example, N-Ar5Ar5-0.6-1.0-3346-3524-4.74x8.00x9.40-100-140.

c) Similarity of the density \( z \)-profiles at the centres between the thermostated regions in a nonequilibrium interfacial system and the same profiles in its corresponding equilibrium interfacial system. We use the systems N-Ar5Ar5-0.6-1.0-3346-3524-4.74x8.00x9.40-100-140 and E-Ar5Ar5-0.6-1.0-3346-3524-4.74x8.00x9.40-120 as an example.
d) Typical \( z \)-dependence of the density \( y \)-gradients; We use the first homophasic nonequilibrium interfacial system as an example, N-Ar5Ar5-0.6-1.0-3346-3524-4.74x8.00x9.40-100-140.

![Graph of d) Typical \( z \)-dependence of the density \( y \)-gradients]

e) Comparison of the Soret coefficient in nonequilibrium interfacial systems of different \( z \)-dimensions and their corresponding nonequilibrium one-phase system

![Graph of e) Comparison of the Soret coefficient in nonequilibrium interfacial systems]

f) Comparison of the locally computed formal Soret coefficients as function of the distance, \( d \), from the Gibbs dividing surface in nonequilibrium interfacial systems of different lengths, \( L_z \); We show only one side of an interface for better readability. The figure gives additionally the Soret coefficient in the corresponding nonequilibrium one-phase system for comparison.

![Graph of f) Comparison of the locally computed formal Soret coefficients]

Figure 54 Detailed analysis of the density distribution in the homophasic nonequilibrium interfacial systems
Figure 55  Equilibrium density distribution to expect in a homophasic nonequilibrium interfacial system; We construct such a distribution by linear interpolation and combination of the density $z$-profiles in several related equilibrium interfacial systems (EISs).
a) Densities as function of $y$ and $z$

b) Comparison of the density $z$-profiles at the centres between the thermostated regions

c) Comparison of the densities as function of $y$ in the phases
d) Comparison of the density $y$-gradients

Figure 56  Example of the density distribution to expect in a nonequilibrium interfacial system based on its related equilibrium interfacial systems; We use the first homophasic nonequilibrium interfacial system as an example, N-Ar5Ar5-0.6-1.0-3346-3524-4.74x8.00x9.40-100-140.

Figure 57  Phase diagram indicating the global states in several differently composed but otherwise comparable nonequilibrium one-phase systems

Figure 58  Concentration dependence of the different density $y$-gradients and of the Soret coefficients in otherwise similar nonequilibrium one-phase systems
a) Nonequilibrium one-phase system; here N-Ar5Ar5-0.6-1.0-6744-223-4.74x8.00x9.40-100-140
b) Homophasic nonequilibrium interfacial system; here N-Ar5Ar5-0.6-1.0-13384-14096-4.74x8.00x37.6-100-140

Figure 59  Particle specific com velocities in selected nonequilibrium one-phase and interfacial systems
Figure 60  Relation between the central particle specific com $y$-velocities, densities and density $y$-gradients at the centres between the thermostated regions in a homophasic nonequilibrium interfacial system
here N-Ar5Ar5-0.6-1.0-13384-14096-4.74x8.00x37.6-100-140
Figure 61  Distributions of selected stress tensor elements using the first homophasic nonequilibrium interfacial system as an example
N-Ar5Ar5-0.6-1.0-3346-3524-4.74x8.00x9.40-100-140
Figure 62  Comparison of the local volume $y$-forces obtained from the normal stresses, $S_{yy}$, and from the shear stresses, $S_{yz}$, in the first homophasic nonequilibrium interfacial system N-Ar5Ar5-0.6-1.0-3346-3524-4.74x8.00x9.40-100-140; The graph shows additionally the $y$-forces from the normal stresses over the same regions as those from the shear stresses to make the similarity more easy to read.

Figure 63  Shear stresses, $S_{yz}$, as function of $z$ in the nonequilibrium interfacial system, N-Ar5Ar5-0.6-1.0-13384-14096-4.74x8.00x36.70-100-140
a) Densities
b) Temperatures
NEMDSimulationThermocapillaryEffectFigures20110925.doc

15-115
c) Com velocities
d) Volume forces
Figure 64  Local densities in the unary nonequilibrium liquid-vapour system
N-Ar5-1.0-8192-4.74x8.00x70.0-110-130
a) **Densities**

- a) **Densities**
b) Temperatures

MeansLocTempYGradZ.eps

MeansLocTempXGradZ.eps

c) Com velocities

MeansLocZComVelZ.eps

MeansLocYComVelZ.eps
Figure 65  Comparison of the local observables in several unary nonequilibrium liquid-vapour systems with different average system temperatures
N-Ar5-1.0-8192-4.74x8.00x70.0-0.110-130, N-Ar5-1.0-8192-4.74x8.00x70.0-0.120-140, and N-Ar5-1.0-8192-4.74x8.00x70.0-0.130-150

Figure 66  Purely repulsive external force field of the type "ff1" in the first solid-liquid interfacial system
N-Ar5-1.0-6870-4.74x8.00x50.0-0.100-140-ff1--4.70---10
a) Densities
b) Temperatures
c) Com velocities
d) Volume forces
Figure 67  Local observables in the first solid-liquid interfacial system with a purely repulsive force field of the type "ff1"
N-Ar5-1.0-6870-4.74x8.00x9.40-100-140-ff1~4.70~10
Figure 68  Intensity of the convection as function of the slope in the first solid-liquid system with an external force field of the type "ff1"
N-Ar5-1.0-6870-4.74x8.00x50.0-100-140-ff1~4.70~--10

Figure 69  Repulsive external force field of the type "ff2" in the unary nonequilibrium interfacial reference system
N-Ar5-1.0-6870-4.74x8.00x9.40-100-140-ff2~1.0~--3.0~10
**a) Densities**
b) Temperatures
c) Com velocities
d) Volume forces
**e) Particle forces**

**Figure 70**  Local observables in the unary nonequilibrium interfacial system with a repulsive force field of the type "ff2", N-Ar1-1.0-6870-4.74x8.00x9.40-100-ff2–1.0–3.0–10
Figure 71  Intensity of the thermocapillary convection in several unary nonequilibrium interfacial systems that differ only in the slope of the external force field “ff2”

Figure 72  Attractive external force field of the type “ff3” in the unary nonequilibrium interfacial reference system, N-Ar5-1.0-6870-4.74x8.00x9.40-100-140-ff3~1.0~3.0~10
a) Densities
**b) Temperatures**
c) Com velocities
d) Volume forces
e) Particle forces

Figure 73  Local observables in the unary nonequilibrium interfacial system with attractive force field of the type "$ff3$", N-Ar5-1.0-6870-4.74x8.00x9.40-100-140-ff3
Figure 74  Intensity of the thermocapillary convection in several unary nonequilibrium interfacial systems that differ only in the slope of the external force field "ff3"

Figure 75  Attractive-repulsive external force field of the type "ff4" in the unary nonequilibrium interfacial reference system
N-Ar5-1.0-6870-4.74x8.00x9.40-100-140-ff4-1.0-3.0-1
a) Densities
b) Temperatures
c) Com velocities
d) Volume forces
e) Particle forces

Figure 76  Local observables in the unary nonequilibrium interfacial system with an attractive-repulsive force field of the type "ff4", N-Ar1-1.0-6870-4.74x8.00x9.40-100-140-ff4-1.0-3.0-1
Figure 77  PT-phase diagram of water

Figure 78  PVT-phase diagram of water
Figure 79  *PT*-phase diagram of the Ar5Ar5 mixture with equimolar composition

Figure 80  Qualitative *P*<sub>T</sub>-phase diagram of the Ar5Ar5 mixture

Figure 81  *PV*-data as obtained in several EMD simulations of an equimolar Ar5Ar5 mixture at different temperatures

Moreover, we give an example of *PV*-data as obtained from the van der Waals equation of state in the wet steam region of a comparable substance.
Figure 82 Examples of unusual stable configurations found in the liquid-liquid-vapour region of the Ar$_5$Ar$_5$ mixture
Figure 83  Example of the concentration dependence of different thermodynamic properties related to the mixing behaviour of the Ar5Ar5 mixture
a) Partial miscibility remote from the critical solution point

b) Partial miscibility near the critical solution point

Figure 84 Examples of "butterfly" diagrams of the Ar5Ar5 mixture

Figure 85 Snap shot of a configuration in the two-dimensional nonequilibrium interfacial system

N-Ar5Ar5-0.6r-1.0-2704-2704-20.0x46.0-60-100
a) Densities
b) Temperatures
c) Com velocities

Figure 86  Local observables in the two-dimensional nonequilibrium interfacial system
N-Ar5Ar5-0.6r-1.0-2704-2704-200x460-60-100