Supplementary Information:

S-shaped Velocity Deformation Induced by Ionic Hydration in Aqueous Salt Solution Flow

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PS1. The simulations results of a system with double length

Simulations with longer slabs are performed to consolidate our results. The new systems are twice the length of the original ones and have the same width and height. The concentrations of the solutions, C1, maintain the same value by doubling the number of water molecules and ions.



Fig. S1 (a) Velocity profiles of the CaCl₂ solution in original system (black) and new built longer system (red). (b) L_s of Ca model series in original system (red) and new built longer system (blue). The dashed line is the original fitted line from Figure 4 in the manuscript.

As shown in Figure S1a, the averaged velocity profile of the longer system is almost the same as the original velocity profile. The calculated data such as L_s is reproduced from the Ca model in this double-length system. The linear dependence of L_s upon the energy density in this new system is illustrated in Figure S1b. It is perfectly within ranges of statistical error bars of the original fitted lines in Figure 5, which implies our numerical calculations are reliable by using the original length in the manuscript.

PS2. The velocity and density profiles of water in the first hydration shells and outside the shells

In order to understand the behavior of water in two parts, i.e., the hydration water in the first hydration shells and other water outside, we calculate their velocities and relative density separately in Figure S2.



Fig. S2 (a) Velocity profiles of hydration water in the first hydration shells (blue), other water outside the first hydration shells (red) and of the entire water (black). (b) The relative density distributions of the entire water and two parts of water. Because the density of the hydration water is one magnitude smaller than the entire water and other water, we plot them in relative densities.

As shown in Figure S2a, the two velocity profiles are quite similar to the velocity profiles of the entire water for most parts, which imply that the hydration shells of ions are flowing along with water. Their differences are belonging to a small quantity of hydration water near the wall, which could be explained by the density distribution. In Figure S2b, The relative densities show that the density distribution of water outside the hydration shell is very similar to the entire water distribution, but the most of hydration water stay in the middle. Only a few of hydration water penetrate into the first layers of water nearest to the walls, they tend to maintain the same velocity with the whole hydration shell which has most part merged in the inner layers. Thus this small parts of hydration water create the difference of the hydration water velocities near the walls, and this difference cause unnoticeable influence on the velocity profile of entire water.

This result implies that the change of the velocity profile does not come from the drag of the hydration shells of ions, but come from the local viscosity changes as described by Eq. 8-10 in the manuscript.

PS3. The structure and the time variation of coordinate number of Ca²⁺ and Na⁺



Fig. S3 The snapshots of the typical structure of the first hydration shell of $Ca^{2+}(a)$ and $Na^{+}(b)$. (c) Radial distribution density of water molecules around Na^{+} and Cl^{-} . (d) Density distribution and relative velocity of water in the vicinity of the Na^{+} cations. The length and direction of the arrow denotes the magnitude and direction of the velocity, and the beginning of the arrow corresponds to the relative position of the unit of flowing water. (e) The time variation of coordination number of water molecules in the first hydration shells of Ca^{2+} and Na^{+} .

As shown in Figure R3, the snapshots of the typical first hydration shells of Ca^{2+} in

Figure S3a and Na⁺ in Figure S3b are illustrated. They are described as layers of hydration water around the ion and consist by the nearest vicinity of the hydration water molecules that interact directly to the ions.

The radius distribution function of water molecules around the ion also provides the structure details of the first hydration shell, such as Figure 2c of the Ca^{2+} in the manuscript and Figure S3c of the Na⁺. The first peak denotes the radius density of the first hydration shell while the location of the first trough denotes the radius of the first hydration shell.

The water density distribution and velocity distribution on the x-z plane around ions also provide us a direct view of the structure and dynamics of the first hydration shells, such as Figure 2d of the Ca^{2+} in the manuscript and Figure S3d of the Na^+ . In Figure S3d, the blue ring around the cation denotes the first hydration shell where the water densely distributed, which is approximately a spherical shell. The relative velocities of the water molecules around the ion are indicated by the red arrows in Figure S3d. They imply that the first hydration shell of Na^+ is whirling around the ion and the structure.

To clarify the dynamical stability of the first hydration shell, we could calculate the time variation of the coordination number in the first hydration shell. It could be calculated by integrating the first peak before the radius R_1 in Figure 2c in the manuscript and Figure S3c here. The time variation of the coordination number of Ca²⁺ and Na⁺ cations are illustrated in Figure S3e. In our simulation, the coordination number of water in the first hydration shell of Ca²⁺ cation is approximately 7.1 and the coordination number of Na⁺ is 4.3, which implies the structure of the first hydration shell is quite stable. Therefore, the dynamical stability of the first hydration shells enables them to provide a stable influence upon the flow behavior of the water molecules.

PS4. The calculations of narrow channel in 1 nm

Simulations of $CaCl_2$ solution and the pure water in a narrow channel in 1 nm are also performed. To keep the same nominal shear rate, the wall velocity is reduced to the half value of the 2 nm system.

As shown in Figure S4a, the new velocity profile of pure water in Figure R4a is far from straight line. It is due to the fact that most water molecules are concentrated near the wall in this narrow channel as shown in Figure S4b, and it leads to the smaller slope in the velocity profile. While in the middle part of the narrow channel, lower water density leads to large gradient of velocity.

For the $CaCl_2$ solution system, velocity changes are milder than the pure water system. Here, the ions and hydration water in the middle would connect the two water layers. The radius of the first hydration shell of Ca^{2+} is about 0.32 nm, so that most of the hydration shells would penetrate into the water layers near the walls.



Fig. S4 (a) Velocity profiles of pure water and $CaCl_2$ solution in the narrow channel in 1 nm. (b) Density distribution of water molecules in the pure water system and the distribution of ions and solvents in $CaCl_2$ solution.

The transport behavior in the narrow channel is quite different from channels larger than 2 nm studied in the manuscript. In the large channels, pure water system behaves with little inhomogeneity. The inhomogeneity in the salt solutions is provided by the presence of hydrated ions. In narrow channels such as 1 nm, pure water system itself would exhibit inhomogeneity due to the size effect, where the channel width is comparable to the size of the water molecules.