

Instant computational tool for laser-induced heat and fluid flows: application to a point-like heat source

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ABSTRACT

A conversion from light to heat, known as a photothermal effect, is an inherent process in optical manipulation because light intensity is highly localized and enhanced in sub-microscale or nanoscale. The heat generated by the photothermal effect in turn induces fluid flows because of thermal convection and/or a thermo-osmotic slip at solid-fluid interfaces. The computation of the temperature variation and the fluid flows is essential to understand the dynamics of dispersed objects. However, the thermo-fluid computation requires certain fluid-mechanics background, posing a barrier for deeper discussions in optical-manipulation community. In this study, an instant computational tool for the temperature and flow fields is introduced. The tool is shared as an open-source code, which is freely available to researchers without a fluid-mechanics background. As a demonstration of the tool, the fluid flows induced by a point-like heat source attached to a substrate, which mimics the situation of plasmonic heating, are discussed in this paper.

Keywords: photothermal effect, thermo-osmotic slip, thermal convection, thermophoresis, optical trapping

1. INTRODUCTION

In optical manipulation such as optical tweezers and plasmonic tweezers, it is necessary to localize light (or electromagnetic fields) to generate optical forces that trap target nanomaterials. In the case of far-field optics, a laser beam is usually focused tightly so that the size of the beam waist is sub-micron order. When plasmonic nanostructures are used, the localization of enhanced electromagnetic fields shrinks down to much smaller nanoscales. Such localized light fields may lead to heat generation due to the absorption of light into materials and/or Joule heating. Resulting localized heat, whose applied region is of the order of micro- and nanoscale in size, then drive fluid motion: a buoyancy force due to the density variation induces thermal convection and a temperature gradient of substrates induces thermo-osmotic slip near solid surfaces [1]. These laser-induced thermal fluid flows, together with inhomogeneous temperature fields, affect significantly the motion of the target nanomaterials in optical trapping. For instance, when the flow is directed toward the trapping site, the probability of having the target in the light-localized region increases, leading to the improvement of optical-trapping performance. However, when the target materials have thermophobic properties, i.e., the targets tend to deplete from a hot part, the optical-trapping performance can deteriorate because of the localized heat.

The thermo-fluid phenomena can hardly be avoided in principle in optical manipulation, although we can try to reduce it more or less, e.g., by using materials with negligible light absorption. Therefore, it is necessary to discuss the temperature and flow fields for the quantitative evaluation on the dynamics of the target nanomaterials. However, the computation of temperature and flow fields necessitates a background in fluid mechanics, which researchers in the field of optical manipulation often lack. Here, we present an instant computational tool to obtain the temperature and flow fields due to laser focusing. The tool is based on the semi-analytical solutions of thermo-fluid equations [2] and is freely available as an open source [3]. In particular, we discuss in this study a possible application of the tool to a typical problem with a point-like heat source.

2. PROBLEM

In Fig. 1(a), we present the schematic summary of the problem that the semi-analytical solution [2] can deal with (see Ref. [2] for the full detail). A fluid is contained in a gap between two parallel substrates, and a focused laser is irradiated in the perpendicular direction to the substrates. The laser is absorbed into the fluid and/or the interface layer (e.g., metal thin films deposited onto substrates) between the fluid and the substrate. Then, the generated heat drives the fluid motion, namely, thermal convection and/or thermo-osmotic slip.

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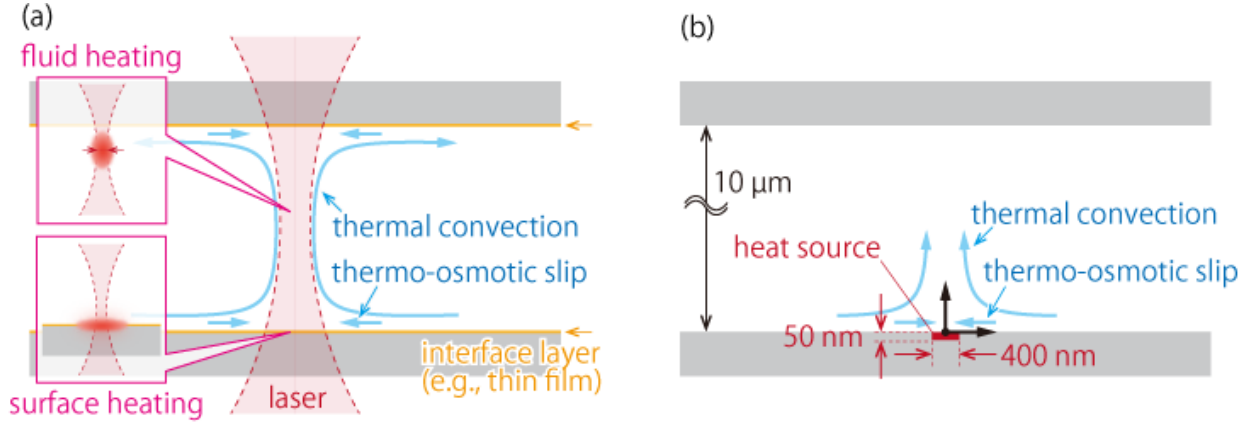


Figure 1. The schematic summary of the problem. (a) The situation that the semi-analytical solution in Ref. [2] can deal with. (b) An example of a point-like heat source presented in this study.

We assume that (i) non-linear effects are negligible and (ii) transport coefficients and physical properties are constant. The assumption (i) indicates that the convection terms in the momentum and energy conservation laws can be neglected and is usually legitimated when we are interested in micro- and nanoscale flows. Under these assumptions, we can linearize the whole system, which allows us to solve the problem semi-analytically via the Hankel transform. To be more specific, the system consists of the heat equations for the fluid and the substrates together with the Stokes equation for the fluid motion. The physical parameters in the semi-analytical solutions are listed as below: the thickness of the fluid layer, the substrates, and the interface layers (i.e., thin films); thermal conductivities of the fluid, the substrates, and the interface layers; the beam power, the beam width, the position of the focal plane, the laser wavelength, the Rayleigh length; the viscosity and the thermal expansion coefficient of the fluid, the absorption coefficients of the fluid and the interface layers, and the thermo-osmotic slip coefficient. Because of the presence of various physical parameters, systematic investigation for all of them is beyond the scope of the present study. The semi-analytical solution [2] is useful since researchers can easily explore by themselves the fluid flow and temperature fields for the parameters they are interested in.

3. RESULTS

To demonstrate the significance of thermo-osmotic slip at the solid-liquid interface, we focus on a typical situation with the plasmonic heating of a single nanostructure as an example. Suppose that a fluid is contained in a gap between two substrates with a distance of $10\ \mu\text{m}$, as shown in Fig. 1(b). At the lower substrate, a laser-absorbing thin film of 50-nm -thickness is deposited. The thermal conductivity of the film is set to same as that of the lower substrate. We irradiate the laser with the beam width of 200 nm at the focal plane to produce a heat in the thin film, as shown in Fig. 1(b). The heat source is small compared with the channel scale and thus can be considered as point-like approximately. Detailed physical parameters were explained in Fig. 11(c) of Ref. [2]. In this paper, we focus on the cases with and without thermo-osmotic slip.

Figure 2 shows the results of the plotting of the semi-analytical solutions. First, panel (a) shows the heatmap of the temperature increase. The generated heat spreads over both the fluid domain ($z > 0\ \mu\text{m}$) and the solid domain ($z < 0\ \mu\text{m}$). The maximum temperature increase is about 30 K at the origin, i.e., $r = 0\ \mu\text{m}$ and $z = 0\ \mu\text{m}$. Note that this maximum value is strongly affected by the absorption coefficient of the film, and thus the detail of the absorption process is required to discuss the temperature field more quantitatively.

Figure 2(b) shows the flow field in the case without the thermo-osmotic slip condition, that is, only the thermal convection is presented, where the temperature field is given in Fig. 2(a). As expected, the flow is induced in the direction toward the heated part near the substrate. However, because of the smallness of the heat source and the narrow gap between the substrates, the magnitude of the flow is of the order of 1 nm/s despite the moderate value of the temperature increase. This is practically negligible and thus we can conclude that the effect of thermal convection is insignificant for the case with the point-like heat source in a microscale confinement.

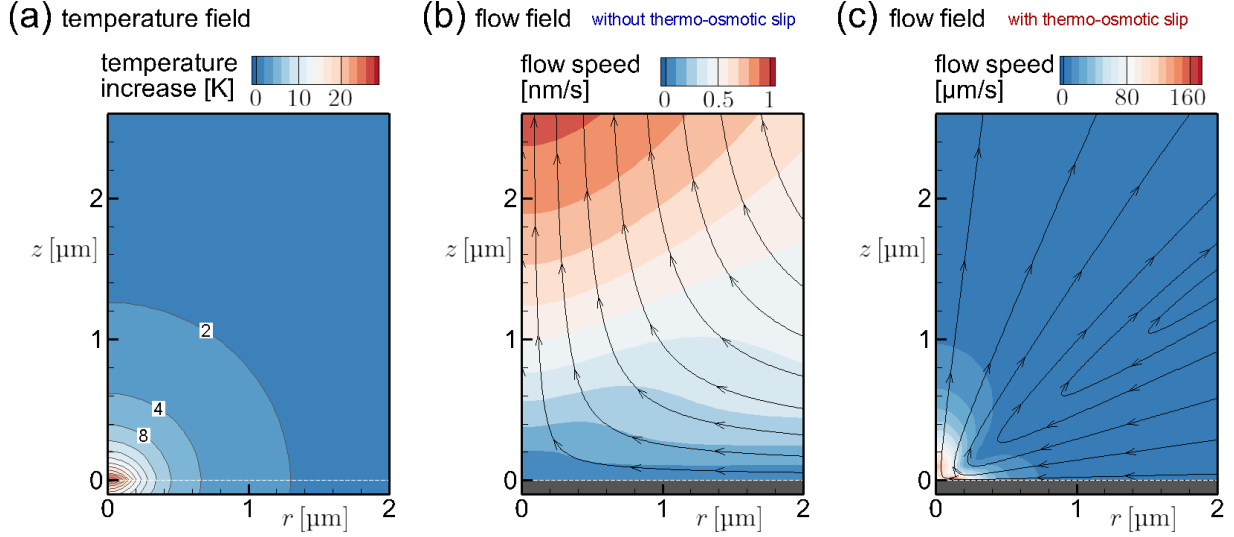


Figure 2. (a) Temperature field and (b,c) flow fields for a situation in Fig. 1(b). A fluid is confined between two substrates with a spacing of $10\ \mu\text{m}$. The laser is focused at $r = 0\ \mu\text{m}$ and $z = 0\ \mu\text{m}$ (i.e., on the surface of the lower substrate). The thin film of the thickness of $50\ \text{nm}$ is deposited on the lower substrate, and the film absorbs the laser to generate heat. The beam radius is set to $200\ \text{nm}$ at the laser focus. Therefore, we can consider that a point-like heat source of the order of $200\ \text{nm}$ is placed at $r = 0\ \mu\text{m}$ on the lower substrate. This situation imitates a typical setting of plasmonic heating. In panel (b), there is no thermo-osmotic slip on the substrates, and thus only thermal convection occurs. In panel (c), the thermo-osmotic slip coefficient is set to $-2\ \mu\text{m}^2/(\text{s K})$, and thus there arises a significant slip flow near the heated part. The physical parameters are the same as those in Fig. 11(c) of Ref. [2] unless otherwise stated.

Finally, Fig. 2(c) shows the flow field with the thermo-osmotic slip boundary condition at the lower substrate. The flow field is qualitatively similar as that of thermal convection in Fig. 2(b), that is, the flow is induced in the direction toward the heated part near the lower substrate. However, using the value of a typical magnitude of the slip coefficient, the flow speed exceeds $100\ \mu\text{m/s}$ near the heated part. As the distance from $r = 0\ \mu\text{m}$ increases, the flow speed decreases, but the speed is still of the order of $1\text{-}10\ \mu\text{m/s}$ at $r \approx 1\ \mu\text{m}$, which is strong enough to transport target nanomaterials from far beyond the laser irradiated region.

4. CONCLUSION

In this paper, we introduced the semi-analytical solution of the temperature and the fluid flows for the photothermal experiment in a confinement between two parallel substrates. As a demonstration of the computational tool given in Ref. [3], the flow fields induced by an approximate point-like heat source were presented, showcasing the significance of thermo-osmotic slip. The computational tool is useful because it does not need numerical simulation with iteration procedures, which are necessary in finite-element methods, providing the information on temperature and flow fields almost instantaneously.

It should be noted that the thermo-osmotic slip coefficient was empirically given in the present computation. Therefore, a theoretical framework to obtain the thermo-osmotic slip coefficient should be developed to control thermally-induced flows for the improvement of the optical-trapping performance.

REFERENCES

- [1] Bregulla, A. P., Würger, A., Günther, K., Mertig, M., and Cichos, F., "Thermo-osmotic flow in thin films," *Phys. Rev. Lett.* 116, 188303 (2016).
- [2] Tsuji, T., Saito, S. and Taguchi, S., "Semianalytical model of optothermal fluidics in a confinement," *Phys. Rev. Fluids* 9, 124202 (2024).
- [3] Tsuji, T., Saito, S. and Taguchi, S., "Instant computational tool of optothermal fluidics," *Kyoto University Research Information Repository* (2024). <https://doi.org/10.57723/287529>