

Phase Inversion in Liquid-Liquid Dispersions

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Background

In a system of two immiscible liquids, usually water (or an aqueous solution) and an organic liquid (e.g. an oil), there are two general types of dispersions which can be formed depending on the conditions of the system. A water-in-oil (W/O) dispersion is a dispersion formed when the aqueous phase is dispersed in the organic phase and an oil-in-water (O/W) dispersion is a dispersion which is formed when the organic phase is dispersed in the aqueous phase. Phase inversion is the phenomenon whereby the phases of a liquid-liquid dispersion interchange such that the dispersed phase spontaneously inverts to become the continuous phase and *vice versa* under conditions determined by the system properties, volume ratio and energy input¹. This is illustrated in Figure 1 below. Thus, by definition, the phase inversion point is the holdup of the dispersed phase for a system at which the transition occurs i.e. when the dispersed phase becomes the continuous phase after an infinitesimal change is made to the system's properties, phase ratio or energy input.

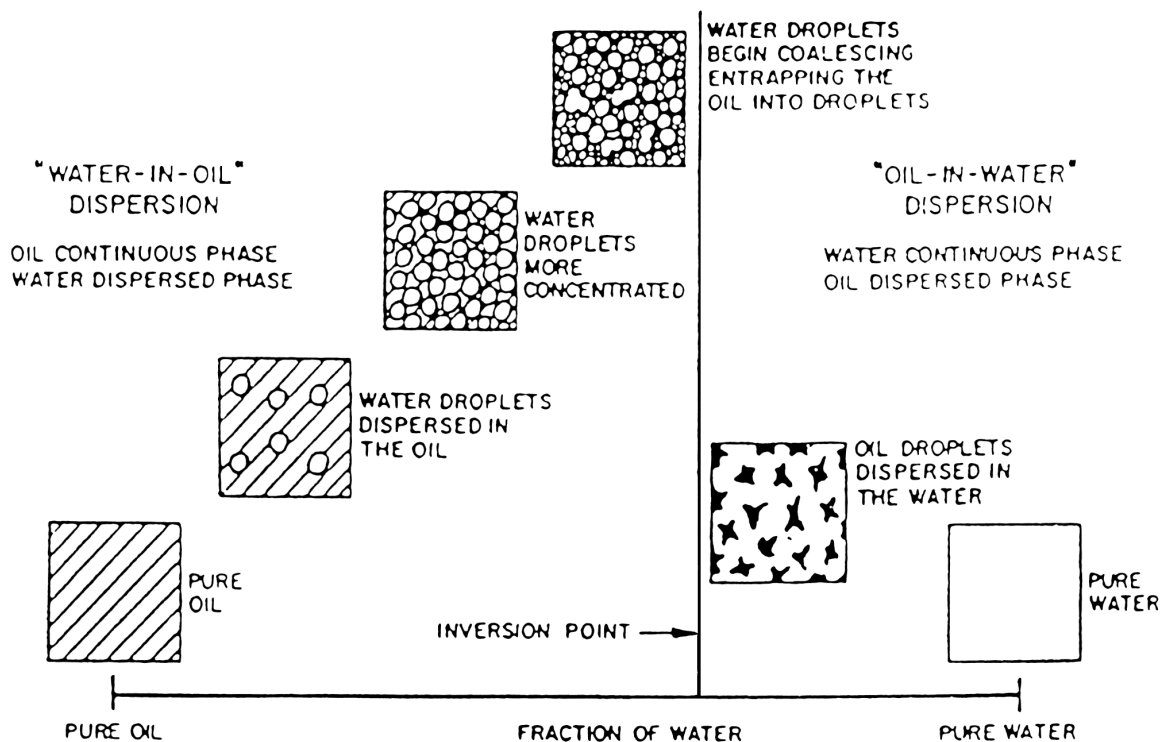


Figure 1 Phase Inversion Process for an Oil-Water Dispersion System (taken from Arirachakaran, 1989)²

Phase inversion can be regarded as a form of the instability of the system, the stability of the dispersion being the least at the point of phase inversion. Phase inversion is thus a very important factor to consider in liquid-liquid extraction since it

can be used effectively in the separation of two immiscible phases. On the other hand, knowledge of the phase inversion point is essential in the preparation of dispersions in order to obtain the desired dispersion. In some operations, spontaneous inversion can be extremely undesirable, especially for mixer-settlers, since the settling times are very different for oil-in-water systems and for water-in-oil systems. Knowing which phase will be the dispersed phase is important in these circumstances. For oil/water flows in pipes, it is important to predict the phase inversion point since it is in this vicinity that the extremes of the pressure gradients will often be found.

Phase inversion behaviour is affected by both the physical properties of the liquids that make up the system as well as the geometric factors of the vessel that the liquids are contained within. Fluid physical properties such as viscosity, density and interfacial tension are among those that affect the phase inversion process. Various geometrical factors such as the agitation speed, the number and type of impellers, the materials of construction and their wetting characteristics are found to influence phase inversion and the ambivalence range. This chapter reviews the work that examines phase inversion with regard to these factors.

Little is known about the detailed mechanism of the phase inversion phenomenon despite the fact that phase inversion has been studied for the past 40 years. In recent years, there has been a revived interest in this area especially for liquid-liquid flow in pipes, because of the abrupt and significant changes that occur in the frictional pressure drop and the rheological characteristics of the dispersion at or near the phase inversion point² (see Figure 2). Nevertheless, much research is still urgently required in order to fully understand the phase inversion process and the mechanisms behind it.

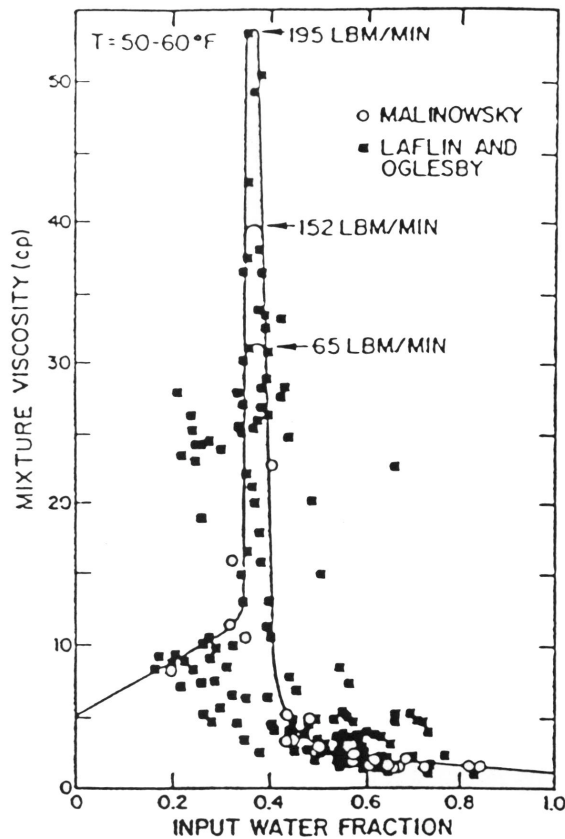


Figure 2 Mixture viscosity as a function of input water volume fraction for low viscosity oils (taken from Arirachakaran, 1989)

Research Objectives

The objectives of this research project are threefold:

1. To study concentrated liquid-liquid dispersions in both agitated vessels and in flows in tubes paying particular attention to the phenomena associated with phase inversion.
2. To bring to bear modern instrumentation techniques and in particular laser photochromic dye tracing, to produce a better phenomenological understanding of phase inversion.
3. To predict the phase inversion holdup in liquid-liquid dispersions by simulating the drop dynamics of coalescence and break-up and to study the various physicochemical parameters affecting phase inversion behaviour.

Experiments

The fundamental difficulty in understanding phase inversion lies in the problem of conceptualising the actual mechanism behind the process. Definitive information on the details of the drop coalescence and break-up processes, which govern the inversion process, remains elusive despite extensive investigations that have been carried out. To gain insight into these processes it is imperative to investigate the system via direct visualisation using non-intrusive flow visualisation methods such as laser photochromic dye tracing. This is carried out by matching the refractive indices

of the immiscible liquid pair and dissolving different photochromic dyes into each liquid phase such that the evolution of the motion of the dispersed and continuous phases at a plane cross-section can be monitored upon irradiation with ultraviolet light. It is hoped that use of Photochromic dye tracing will provide experimental data as well as insight with which to advance and ultimately validate theoretical predictions obtained in the Modelling component of this project.

Modelling

Few computational models have been developed for predicting phase inversion. Juswandi³ reports a stochastic model, which attempts to simulate phase inversion. In his model, a similar algorithm to the Metropolis Monte Carlo algorithm^{4 5} is used to generate a trajectory in phase space, which samples from a chosen statistical ensemble. This constitutes the random motion of the drops within the dispersion lattice. Similar pseudo-random number generators are also used to determine the likelihood of drop break-up in the system as well as to select drops at random as candidates for the break-up process. Our work attempts to overcome the limitations found in Juswandi's model and to incorporate the fundamental processes of drop hydrodynamics^{6 7}, which are, absent in the existing model. Since a large portion of phase inversion research has been concentrated on liquid-liquid dispersions in agitated vessels (thereby resulting in a vast amount of experimental data in this field) the code was adapted to model a dispersion that occurs in agitated vessels^{8 9}. This step is necessary for the validation of the code before attempting to model flows of concentrated liquid-liquid dispersions in pipes. In future, we hope to utilise novel techniques such as Lattice Gas Automata and Lattice Boltzmann methods¹⁰ to provide a more faithful representation of the hydrodynamics and thus a more accurate description of the system.

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