



Building an e-Print Service: Addressing the Social Challenge in Environmental Management Science

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SCIENTIFIC COMMUNICATION IS CHANGING

Researchers need access to
programmatic and
interdisciplinary research



Results are
needed more
quickly

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ASSESSMENT OF NEPHELINE PRECIPITATION IN NUCLEAR WASTE GLASS THERMOCHEMICAL MODELING

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ABSTRACT

A thermochemical representation of the Na-Al-Si-B-O system relevant for nuclear glass has been developed based on the associate species approach for the glass solution model. Thermochemical data were assessed and associate species data determined for binary and subsystems in the Na₂O-Al₂O₃-B₂O₃-SiO₂ system. Computed binary and ternary phase diagrams were compared to published diagrams during this process, with adjustments in data made necessary to obtain consistent thermodynamic values. The resulting representation for the oxide system was used to help understand the problem of nepheline precipitation in certain glass formulations.

INTRODUCTION

High-level nuclear and transuranic wastes are currently foreseen as being incorporated into a host glass for permanent disposal. A large number of glasses have been explored, with borosilicate glass as the typical base composition. Glass compositions are under development at Pacific Northwest National Laboratory (PNNL) and Savannah River Laboratory that will dissolve the waste species in a glass matrix. Issues of glass stability are important in that the glass must remain mechanically intact and retain a low leach rate on exposure to moist environments. A somewhat opposing goal is to maximize waste loading of the glass, with a significant economic gain associated with incremental increases in waste content.

A problem identified at PNNL is the precipitation of a nepheline phase (Na₂O·Al₂O₃·2SiO₂) within certain compositions during the cooling of glass, which weakens the network structure by removing the glass formers Al₂O₃ and SiO₂. The result is that nepheline precipitation in high-level waste glass limits waste species loading. It has been observed that compositions rich in Al₂O₃ and Na₂O are particularly prone to precipitating nepheline [1]. The rapid kinetics of nepheline formation in the cooling glass suggests that an equilibrium thermodynamic model may provide useful insights with regard to the composition parameters governing its precipitation [1]. Currently, there are limited thermochemical models for complex glass compositions, with much of the guidance for glass chemistry based on empirical or semi-empirical approaches. In the work reported in this paper, a thermochemical model for the Na₂O-Al₂O₃-B₂O₃-SiO₂ crystalline and glass system has been developed and applied to the problem of nepheline precipitation.

SOLUTION MODEL

An associate model developed in the 1980s was used to represent the thermochemical

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Phase Inversion Studies in Liquid-Liquid Dispersions

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A study of the phase inversion behavior of liquid-liquid dispersions in stirred vessels is performed for liquids of various physical properties at various operating conditions. Physical parameters studied are density (867 to 1180 kg/m³), viscosity (0.00096 to 0.00378 Pas), and interfacial tension (0.0089 to 0.0323 N/m). Ambivalence region plots are presented and compared with results reported in the literature. Experiments are performed to examine the effects of impeller type and impeller-to-tank diameter ratio (*D/T*) on the ambivalence behavior. Also, phase inversion time experiments are performed to investigate the time required for complete phase inversion under various dynamic conditions. The traditional method of plotting the organic phase volume fraction at phase inversion against the agitation speed at that condition is compared with the method of plotting the initially dispersed phase volume fraction at phase inversion against the agitation speed at that condition. A hysteresis phenomenon is shown in phase inversion from *OW* to *WO* and *WO* to *OW* dispersions. Also, it is shown that, depending on the physical properties of the dispersed and continuous phases, phase inversion may occur when the agitation speed is increased or decreased.

On a menée une étude du comportement d'inversion de phases de dispersions liquide-liquide dans des réservoirs agités pour des liquides aux propriétés physiques diverses et dans différentes conditions de fonctionnement. Les paramètres physiques étudiés sont la masse volumique (867 à 1180 kg/m³), la viscosité (0,00096 à 0,00378 Pas) et la tension interfaciale (0,0089 à 0,0323 N/m). Des relevés des régions d'ambivalence sont présentés et comparés aux résultats de la littérature scientifique. Des expériences sont menées afin d'examiner les effets du type de turbine et du rapport du diamètre de la turbine au diamètre du réservoir (*D/T*) sur le comportement d'ambivalence. De même, des expériences sur les temps d'inversion de phase sont menées pour connaître le temps requis pour une inversion de phase complète dans des conditions dynamiques variables. La méthode traditionnelle de trace de la fraction volumique de la phase organique à l'inversion de phase par rapport à la vitesse d'agitation à cette condition est comparée à la méthode de trace de la fraction volumique de phase dispersée initiale à l'inversion de phase par rapport à la vitesse d'agitation à cette condition. Un phénomène d'hystérèse est montré dans l'inversion de phase des dispersions *OW* à *WO* et *WO* à *OW*. On montre également que, selon les propriétés physiques des phases dispersée et continue, l'inversion de phase peut survenir lorsque la vitesse d'agitation est augmentée ou diminuée.

Keywords: liquid-liquid dispersions, phase inversion, ambivalence region, hysteresis.

In a stable liquid-liquid dispersion there is a dynamic equilibrium between the two competing phenomena of drop breakage and drop coalescence. The breakage of drops is due to turbulence created by the impeller. Cutter (1966) found that the fraction of the small eddies which cause drop breakage was largest in the immediate vicinity of the impeller, and a study by Tsouris and Tavlariades (1994) led to the conclusion that drop breakage is confined to the impeller region. Drop coalescence is thought to occur everywhere in the vessel (Calabrese et al., 1986).

If the system deviates from this equilibrium in a manner which causes the drop coalescence rate to greatly exceed the drop breakage rate, there will be a rather sudden coalescence of the dispersed phase drops into a single continuum; and the phase which was previously continuous will become dispersed. This phenomenon usually occurs within a few seconds and is known as phase inversion.

The post phase inversion dispersion may be quite different from the initial dispersion with respect to dispersed and continuous phase physical properties, but the rates of drop breakage and coalescence are once again at equilibrium.

Phase inversion is among the least understood phenomena in liquid-liquid systems. An understanding of phase inversion often dictates that they be operated at high dispersed phase volume fractions and a high degree of agitation to ensure sufficient interfacial contact between the phases. Operation under such conditions, if not properly controlled, is always performed at the risk of the occurrence of phase inversion. The phase inversion behavior is affected by the physical properties of the liquids which constitute the dispersion as well as by geometric factors such as the type and number of impellers and materials of construction of the agitator and vessel. Effects of various physical properties, such as density, viscosity, interfacial tension, and droplet surface charge, have been examined by several investigators (Quinn and Sigloh, 1963; Selker and Steicher, 1965; Luhnig and Sawistowski, 1971; McClure and Mansoori, 1978; Gutlinger et al., 1988; and Tobin and Ramkrisna, 1992).

Other investigators have studied the effects of geometric parameters. For example, Gilchrist et al. (1989) showed that the spacing between the baffles and vessel wall can affect drop coalescence at low agitation speeds. Kumar et al. (1991) examined the effects of the material of construction of the impeller on phase inversion behavior. They found that, if the materials of construction of the impeller were essentially coated by the dispersed phase, the drop coalescence rate was significantly reduced.

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CHALLENGES IDENTIFIED AT THE OUTSET

- ***Identifying the scope***
- ***Obtaining contributions from scientists***
- ***Working across agencies***

CHALLENGE: Setting the Scope

- What is environmental management science?
- What resource types should be included?
- How old could the material be?
- How to handle the “aging” of the content?
- How should the e-Prints relate to other products and services?

e-PRINT TEAM RESPONSE: Setting the Scope

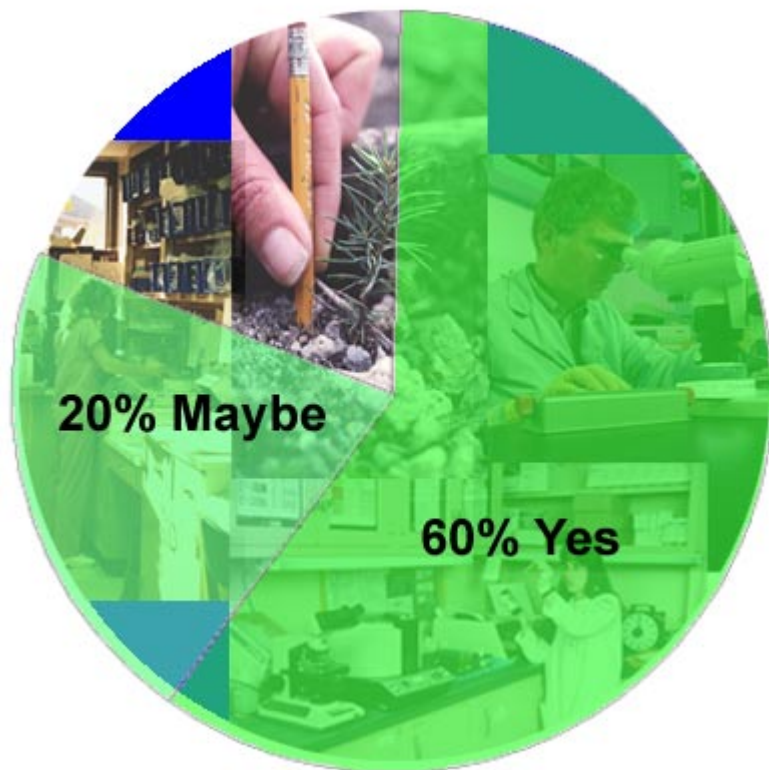
- Core from EM researchers, including technical reports
- Government information from partners
- Manuscripts, reprints, white papers, presentations, posters, etc.
- Manuscripts preferred because of copyright issues
- Emphasizing current material
- Collections allow contributions to be segmented in different ways

CHALLENGE: Obtaining contributions from scientists

Would scientists contribute?

- Intellectual property and copyright issues
- Concerns about prior publication
- Early sharing across agencies is not part of the culture

RESEARCHERS SUPPORT e-PRINT SERVICE



Both EMSP and EPA/ORD researchers were surveyed during 1999.

Overall, 80% of survey responses were favorable

BENEFITS OF e-PRINT SERVICE IDENTIFIED BY RESEARCHERS

- Increases access to environmental management science research
- Increases visibility of results and investigators
- Facilitates communication across agencies and between researchers
- Potentially increases research productivity
- As a by-product, increases public access to government produced or sponsored information

e-PRINT TEAM RESPONSE: Obtaining Contributions

- Let the researchers decide what to contribute
- Access limitations controlled by the contributor
- Established partnerships with agencies to give researchers high level incentive
- **PROMOTION, PROMOTION, PROMOTION**
 - Quarterly newsletter
 - Contributor instructions on Web page
 - Attendance at scientific meetings

CHALLENGE: Working Across Agencies

- Agencies want visibility
- Some have no funding or resources to provide
- Different approaches to technical issues

e-PRINT TEAM RESPONSE: Working Across Agencies

- Provide for various roles that organizations can play
- Ensure visibility while maintaining a single look
 - developed a non-agency logo
 - identify the agency source when the results are presented
- Central repository provides consistency in metadata

CONCLUSIONS

- Identifying social and cultural challenges early is important
- Challenges will remain for a long time
- Goal of turning the challenges into opportunities



- Contributions are welcome and new partners are encouraged
- Demo available at Booth # 1201
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