

Boiler Water Deposition Model

Part 1: Feasibility Study



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Technical Report

Boiler Water Deposition Model

Part 1: Feasibility Study

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Final Report, December 2004

EPRI Project Manager
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PRODUCT DESCRIPTION

Many sources of availability and performance losses in fossil units involve deposition on water- and steam-touched surfaces, with the most acute effects occurring in boilers and turbines. Earlier deposition state-of-knowledge assessments sponsored by EPRI established three broad classifications of deposition phenomena (EPRI reports 1004194 and 1004930). However, within these classifications are many processes and influencing factors that need to be considered in order to make meaningful improvements in deposition control. Enhanced understanding of deposition in boilers was determined to be the greatest source of benefits and value to end users. To help realize such benefits, EPRI has sponsored this feasibility study on modeling the various processes governing deposition in fossil boilers.

Results & Findings

The purpose of this feasibility study is to identify, review, and critically assess several existing models that could be considered during construction of an aggregate model specific to high pressure fossil boilers. Included are discussions of model input, intermediate and output parameters, assumptions, limitations, and applications experience. Although many of the models considered were developed for application to nuclear cycles, such models frequently appear relevant to fossil boilers. This feasibility assessment has shown that establishment of an aggregate deposition model specific to fossil plant boilers should be possible. An overall strategy to construct the model and address information needs has been formulated.

Challenges & Objective(s)

The overall objective of this project was to examine the feasibility of developing a comprehensive or aggregate model for deposition processes in fossil boilers of conventional cycles by combining known models relating deposition to heat transfer, mass transfer, solubility, and other relevant mechanisms. The goal of model development activity is to create a tool that will apply to new and existing fossil units to better manage any deposition that cannot be avoided and thus eliminate or minimize the negative impacts of deposition on performance and profitability. The complexity of deposition is significant; integration of fossil boilers requires the coordinated efforts of many technical specialists. Because of these factors, model development will be done using a phased approach.

Applications, Values & Use

The next step in formulating a useful boiler water deposition model is to develop an initial version of the aggregate model following the approach described herein. After this has been accomplished, model testing and refinement activities will be required. EPRI envisions that the final version of the model will be used for several purposes. The first purpose will be to support parallel project activity intended to improve the understanding of boiler corrosion processes. The second will be to establish improved criteria for determination of when operational chemical cleaning of boilers is required. Finally, creation of a suitable aggregate model on deposition in fossil boilers will support future refinement of existing guidelines for fossil plant cycle chemistry.

EPRI Perspective

Boiler tube failures (BTFs) have consistently been cited as the number one source of availability loss in fossil units. BTF mechanisms involving deposition on boiler waterside heat transfer surfaces are a significant concern at many plants. Research directed towards an improved understanding of boiler deposition is regarded as integral to improving fossil unit BTF and availability statistics.

Approach

The project team examined the possibility of developing a comprehensive model for deposition processes in fossil plant cycles by combining known models, which generally focus on limited and specific aspects of deposition. This was accomplished by review of previously published models and other assessments of deposition phenomena with possible relevance to deposition in fossil boilers. In addition, a colloquium of several leading experts in this area was convened to document their activities and solicit their views on development of the aggregate model.

Keywords

Deposition
Fossil Plant Availability
Turbine Deposits
Cycle Chemistry

ABSTRACT

Many of the chemistry related availability and performance losses in fossil units involve deposits on water and steam touched surfaces. Prior state-of-knowledge assessments have shown that all areas of fossil steam-water cycles may be adversely impacted by deposits, with the most acute effects occurring in boilers and turbines. Three broad classifications of deposition phenomena were established. Boiler deposition was identified as the area of broadest concern to the industry; an improved understanding of deposition in boilers was determined to be the greatest source of benefits and value to end users. These studies also identified a number of factors that influenced deposition activity and revealed the complex nature of the physical and chemical processes governing deposition. In view of these findings, it was concluded that modeling of deposition in fossil boilers should be pursued and that application of knowledge applied to develop other models focusing on specific phenomena could result in establishment of an integrated or aggregate model that addresses the various physical and chemical processes involved.

The purpose of this feasibility is to identify, review and critically assess several existing models that could be considered during construction of an aggregate model specific to high pressure fossil boilers. Included are discussions of model input, intermediate and output parameters, assumptions, limitations and applications experience. Although many of the models considered were developed for application to nuclear cycles, such models frequently appear relevant to fossil boilers. The study concludes that establishment of a useful aggregate model should be feasible. A general approach to follow in constructing, evaluating and refining the model is presented.

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1

INTRODUCTION AND BACKGROUND

1.1 Background

The presence of deposits, within and on the heat transfer surfaces of equipment comprising the steam/water cycles of fossil plant units, has been noted since the very beginning of the commercial steam and power generation industry. Deposits can form at nearly all locations within the steam-water cycle. However, experience makes it clear that the operational and resultant economic impacts of deposition vary significantly by location.

Advancements in unit design, specifically increased operating pressures, higher heat fluxes in boilers and cycles with higher thermal efficiencies, have resulted in increased emphasis on equipment cleanliness, requiring careful attention to operation and maintenance practices. The influence of the cycle chemistry on deposition activity has long been recognized, as has the role of deposition as an integral part of mechanisms that cause damage and produce failures in pressure parts in contact with water and steam. The area of greatest concern to fossil plant personnel is in boiler tubes and turbines, where failures can have substantial negative impacts on unit availability and reliability. However, deposition occurs at other locations in the steam-water cycle as well, and these deposition events also affect unit performance.

Deposition consists of three general processes: ^(1,2)

1. Physical attachment of suspended and colloidal solids to surfaces.
2. Formation of solids from low solubility impurities present in the water or steam on component surfaces, including reversible deposition phenomena collectively referred to as “hideout” and “hideout return” activity.
3. Deposition processes that are related to surface phenomena including adsorption, absorption and ion exchange on surfaces.

Factors or parameters known or believed to be related to the basic deposition process categories and mechanisms were previously identified and ranked. ^(1,2) A team of cycle chemistry experts was convened in 2002 to discuss various aspects of the state of knowledge. Parameters considered relevant to each process group were ranked according to approximate influence on generation and deposition within condensate systems, feedwater systems, boiler waterwalls, superheaters and reheaters and steam turbines. In 2003, the team assembled details on these parameters for use in evaluating the feasibility of developing a model of deposition specific for fossil plants. This model would include both drum and once-through type boilers.

Introduction and Background

Over 40 parameters and factors that influence deposition were identified under Part 1. Although no additional parameters were identified under Part 2, significant additional information and mathematical relationships were reviewed and summarized for later use in modeling the deposition process. The highest ranked parameters were found to be transient conditions (startup, shutdown, load changes, etc.); concentrations of impurities (contaminants), oxidizing agents (oxygen) and particles; pH at operating temperatures; mass transport; condensate polishing and filtration; chemical treatment; temperature; boiling, condensing and flow regimes; agglomeration of particles; stream quality (moisture); pressure; tube/surface and oxide/hydroxide compositions and interactions; time; steam/water properties; heat flux; size and shape of particles; corrosion rate; configuration of hardware and zeta potential. Key parameters were selected from the long list based on their apparent, even if not fully understood, influence on one or more of the three deposition process types. These key parameters are (a) dynamics of deposition and release (as it affects both boilers and turbines), (b) heat flux (primarily in boiler waterwall tubes), (c) mass transport, (d) solubility in steam and water and (e) surface finish (primarily in turbines and steam generator water tubes). Additional parameters of interest were also identified for possible further study.

1.2 Objective

The objective of this project was to examine the possibility of developing a comprehensive model for the deposition processes in fossil plant cycles by combining known models relating deposition to heat transfer, mass transfer and steam solubility. The goal of the model development is to create a tool that would apply to new and existing fossil units to better manage any deposition activity that cannot be avoided and, in so doing, eliminate or minimize the negative impacts of deposition on performance and profitability. This development would be done in several phases.

1.3 Approach

The study considered three general categories of deposition:

- Deposition of insoluble (particulate) material,
- Deposition of soluble material and
- Absorption.

The key transport and deposition parameters considered in the feasibility study included, as a minimum, the following:

- Dynamics of Deposition and Release (as it affects both boilers and turbines),
- Heat Flux (primarily in boiler waterwall tubes),
- Mass Transport,
- Solubility/Steam,
- Solubility/Water and

- Surface Finish (primarily in turbines).

Additional parameters of interest, for which more information is needed to establish their role in fossil plant units and determine their impact on possible solutions to deposition problems, include the following:

- Agglomeration of Particles,
- Catalysis,
- Electrical Charging of Water,
- Electrochemical Potential and Oxidation Potential (ECP/ORP),
- Ion Exchange Properties of Metal Oxides,
- Magnetic Properties of Solids, Surfaces and Deposit/Oxide and Electromagnetic Fields,
- Molecular Cluster Collisions,
- Particle Size Distribution,
- Porosity (and Density) of Deposits and Oxides,
- Steam/Water Boiling and Condensing Regimes,
- Steam/Water Flow Regimes,
- Steam/Water Properties,
- Transport of Soluble Material and Impurities on Particles by Ion Exchange, Adsorption, Absorption and Magnetic or Electromagnetic Attraction and
- Zeta Potential (ZP).

The project consisted of five tasks:

Task 1 – Evaluation of Existing Equations and Models

The first task consisted of collecting and reviewing the current literature on existing data, equations and models to address the effects heat flux (primarily in boiler tubes), mass transfer mechanisms (in boiler tubes and turbines) and steam/water solubility on deposition. Each of the identified models is considered a module for the proposed aggregate model, if such an aggregation is possible.

This task focused on four categories:

- Heat Transfer Equations and Models
- Mass Transfer Equations and Models
- Solubility Equations and Models for Steam and Water
- Particle Equations and Models for Corrosion Products

Introduction and Background

The result of this literature search was a list of key input and output parameters, including the ranges of those parameters. Another important aspect of this task was the identification of variables on which the key input parameters depend. This was a first step toward identification of overlapping parameters.

A colloquium of experts was convened as part of this task to identify and discuss available equations and models that may be useful in developing a comprehensive, aggregate model of deposition in critical components in fossil power plants. The foci of this effort were the boiler and turbine. Notes from the colloquium are contained in Appendix A.

Task 2 - Document Assumptions, Limitations and Input/Output Parameters

For each of the four model categories (as defined in Task 1), the input and the output parameters were identified, and the major assumptions and limitations of the models were evaluated.

Task 3 - Identify Overlapping Input/Output Parameters

Overlapping input and output parameters were identified for each model or set of equations to determine the ability to merge the independent modules into a comprehensive model. The output parameters could compliment each other, extending the characterization of the deposition, or refer to the same output parameter, identifying a conflict in the output.

Task 4 - Identify Missing Data or Equations

Probable areas were identified where the feasibility of interconnection between modules may pose a problem because of missing data or models. The impact of this missing information on the success or enhancement of the comprehensive model was identified. Also, any lack of available data or constants for application to fossil plants was identified.

Task 5 - Identify Portions of Selected Models for Future Development

Portions of the selected models and equations were identified for possible future development based on this feasibility study. However, since the feasibility study was not an exhaustive review of the literature, it may be expected that additional models and equations may be identified as the development proceeds.

1.4 Report Overview

This report supplements work that was performed in 2002 and 2003 on the state-of-knowledge on deposition in fossil plants. Additional details on parameters that influence deposition can be found in the earlier reports.^(1,2) Section 1 of this report provides information on background and objectives. Section 2 of this report contains an assessment of 34 sets of data, equations and models that were used to assess the feasibility of an aggregate model. Most of Section 2 utilizes empirical or semi-empirical information plus some fundamental equations. Appendices A and B supplement the results of the assessment in Section 2, including the results of a colloquium that was sponsored under this project (Appendix A) and a review of relevant fundamental equations

(Appendix B). Each individual set of data, equations and models is reviewed separately in Section 2. Then, all of the required input and output parameters (including coefficients and intermediate output parameters) from Section 2 are reviewed collectively in Section 3, and conclusions and recommendations are provided in Section 4. Sections 5 and 6 are a list of references and a bibliography, respectively.

2

RESULTS

2.1 Colloquium on Modeling Deposition

A small group of industry experts on deposition assembled at the Colloquium on Modeling Deposition in Boilers of Fossil Fueled Power Plants on January 28 - 29, 2004 at the Electric Power Research Institute (EPRI) office in Charlotte, NC to identify and discuss available equations and models that may be useful in developing a comprehensive, aggregate model of deposition in critical components of fossil power plants. The foci of this effort were the boiler and turbine. Details from this colloquium are given in Appendix A and summarized in the following text.

Several presentations contained examples of successful first, principle and empirical models that were simple. Models for particulate material did not contain extensive equations with elaborate solutions. Additionally, suggestions for complimentary models and equations were given by the presenters. The group concluded that model development would need to be done in a step-wise manner and should include both experimental and field data that are as close to the modeled phenomena as possible. Model development with regard to boiler waterwall surfaces should consider individual plant types, as follows:

- Subcritical plants with boiler tube failures (BTF),
- Subcritical plants without BTF,
- Supercritical plants with oxidizing chemistry and possibly
- Supercritical plants with reducing chemistry.

The boiler models and equations are primarily applicable to subcritical units. The turbine model is applicable to subcritical and supercritical units.

Missing data and the potential complexity of an aggregate model were seen as impediments. Also, detailed thermal-hydraulic performance models, necessary for modeling the local deposition phenomena, may be proprietary.

2.2 Detailed Evaluation of Existing Equations and Models

Numerous sets of data, equations and models were identified. This information was separated into four primary categories for the purpose of evaluating the interrelationships of dependent and independent variables. These categories are as follows:

Results

- Heat transfer equations and models
- Mass transfer equations and models
- Solubility equations and models for steam and water
- Particle equations and models for corrosion products
- Mixed equations and models

The categories are not independent and, at times, were difficult to categorize because of the interrelationships. The results clearly show the complex interdependence and provide a framework for combining available equations and models. The mixed category was used when significant information was available for more than one of the four major categories. Over half of the sets of data, models and equations were placed in the mixed category.

The text in Sections 2.2.1 – 2.2.5 summarizes a detailed assessment of 34 sets of data, equations and models for each of the categories. Section 2.3 contains a less detailed assessment of additional equations and models.

2.2.1 Heat Transfer Models and Equations

2.2.1.1 Time Dependent, Heat Transfer

Deposition Mechanism: Insoluble Material

Source: Povarov and Petrova,⁽³⁾ Part 1 of 2

Description: This model was designed to predict the deposition rate of insoluble material (colloidal and suspended solids) as a function of heat flux.

Assumptions: Models are valid only for heat flux that was tested.

Successful Applications: This model has been successfully applied to several sets of data.

Limitations: Constants given for iron and copper only. Equations apply only to insoluble material. Mass transfer and heat flux equations are provided, but they are not connected to each other. A noted significant impact of enthalpy is not addressed in the equations.

Significant Application Observations: Although zeta potential is cited as having a significant influence on the exponent applied to the heat flux for iron (not discussed for copper), the data presented appear to show minimal impact of electrophoretic effects compared to heat flux and concentration. Copper becomes significant when heat flux exceeds 200 kW/m² (440 BTU/hr/in²). With oxygenated treatment, the inner layer (~0.5 micron or ~0.019 mil thick) was more dense than the outer layer (0.6-1 micron or 0.023-0.039 mil). Water treatment impacts thermal conductivity by a factor of 2-3.

Possible Refinements: Assess the data, showing porosity as a function of fluid temperature, to determine if porosity should be included in equations (not currently included by authors). Assess the connection between electric field potential, heat flux and other parameters discussed by authors.

Assessment for Fossil Plant Application: Iron data were collected under field conditions for supercritical and subcritical conditions in boilers.

Output Parameter(s): Deposit Rate for Solids (0-0.015 mg/cm²-hr or 0-2.12x10⁻⁷ lbm/in²-hr or Iron and 0.0001-0.0017 mg/cm²-hr or 1.419x10⁻⁹-2.412x10⁻⁷ lbm/in²-hr for Copper)

Input Parameters:

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Time	None	Iron: Up to 9,000 hours Copper: Not Cited	None	None
Heat Flux	None	Iron: 50-500 kW/m ² (110-1,100 BTU/hr-in ²) Copper: 300 kW/m ² (660 BTU/hr-in ²)	Zeta potential (Cited Only for Iron)	Zeta potential Impacts Exponent on Heat Flux Over a Range of 1-3.5.
Concentration (Bulk) of Depositing Material	Iron and Copper	Iron: 0-1 ppm Copper: Up to 15 ppm - With 3.5-5 ppm Iron	None	Iron: Concentration of Soluble Iron is Total Minus Insoluble Copper: Equation Needs Ratio of Ionic and Non-Ionic Copper
pH	None	Copper: pH = 10.8	None	Parameter Not Included in Equations
Phosphate	Mixture of Various Forms of Phosphate	Copper: 100 ppm phosphate	None	Parameter Not Included in Equations

Results

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Temperature	None	Iron: 100-316°C (212-601°F) and Up to 565°C (1049°F) Copper: Not Cited	None	Parameter Not Included in Equations
Pressure	None	Iron: Up to 263 kg/cm ² (255 atm, 3750 psi) Copper: Not Cited	None	Parameter Not Included in Equations
Deposition Constants	Depends on Composition (Iron and Copper and Other Components)	Iron: 5.7 x 10 ⁻¹⁴ Copper: Not Cited	Not Cited	Constant for Iron or Copper
Thermal Conductivity	Composition of Deposit	3-5 W/m-K (2.2-3.7 BTU/hr-in-°F) for Non- Boiling and 10-35 W/m-°K (7.4-26 BTU/hr-in-°F) for Boiling	Temperature	Equations are given for thermal conductivity, but the equations are not connected by the authors to the heat flux equations.

2.2.1.2 Time Dependent, Heat Transfer (Convection)

Deposition Mechanism: Soluble Material**Source:** Mann and Castle⁽⁴⁾

Description: This work was designed to assess the concentrating of materials in a crevice, having the geometry similar to a nuclear steam generator tube-to-tubesheet crevice. The crevice was packed with carbon. Results appear to be similar to the convection term of Cleary, *et al.*⁽⁵⁾

Assumptions: A simple diffusion model will describe the concentrating of salt in a crevice.

Successful Applications: Applied to a graphite packed laboratory test apparatus.

Limitations: Solution was maintained at atmospheric pressure boiling point. Only limited bulk chemicals were tested (sodium nitrate and sodium chloride).

Significant Application Observations: Salt accumulated at a constant rate until an equilibrium concentration was reached, and, then, the net accumulation diminished to near zero. At constant temperature, the rate of accumulation decreased exponentially as equilibrium was approached. Equilibrium was reached within a few hours at a constant input concentration. Conversely, salt was released within a few hours after reducing the bulk concentration to zero.

Possible Refinements: None

Assessment for Fossil Plant Application: The simple model has merit for localized accumulation of soluble chemicals within a deposit.

Output Parameter(s): Mass of Salt Deposited (1.3-3.5 mg or $2.9-7.7 \times 10^{-6}$ lbm), Mean Concentration Factor (700-3,600), Rate of Salt Accumulation (0.315-31.5 mg/hr or 6.9×10^{-7} - 6.9×10^{-5} lbm/hr)

Input Parameters:

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Time	None	Up to 60 Hours	None	Steady State Concentration Reached within 30 Hours or Less
Heat Flux	None	85-230 kW/m ² (187-506 BTU/hr-in ²)	Length, Power and Surface Area	None
Temperature Above Boiling Point of Water	Dependent on Chemical Being Concentrated	34-90°C (61-162°F) Above Boiling Point of Water	None	Not a Direct Input Parameter to the Equations
Density (Water)	None	Not Cited	Temperature and Pressure	None
Latent Heat of Vaporization	None	Not Cited	None	None
Salt Concentration in Bulk Water (Feed to Crevice)	None	12-120 ppm	None	Not a Direct Input Parameter to the Equations
Volume of Bulk Solution	None	128-131 mL (4.32-4.42 oz)	None	None

Results

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Volume of Pores	None	1.45 cm ³ (0.088 in ³)	None	None
Volume of Crevice	None	100 mm ³ (0.0061 in ³) for a gap of 0.03 mm (0.012 in) and 56% porosity	None	Not a Direct Input Parameter to the Equations
Porosity	None	47%	None	Not a Direct Input Parameter to the Equations

2.2.1.3 Steady State, Heat Transfer

Deposition Mechanism: Insoluble Material

Source: Kaar, *et al.*⁽⁶⁾

Description: This model was designed to describe heat conduction through layered deposits using the Krisher model that is a derivative of the Maxwell model of heat conduction in composite materials. This model describes the method of combining thermal resistances of several layers by combining two simple models of alternating plate components (layers) that have pores perpendicular and parallel to the heated surface. This is done to describe (a) active layers that have chimneys and capillaries and (b) inactive layers that no longer have chimneys and capillaries. Active layers have pores that are parallel to the heat flux, and inactive layers have pores that are perpendicular to the heat flux. Active layers produce steam within the deposit.

Assumptions: In each of the layers, porosity is constant. The bulk mass flow is perpendicular to the heated surface.

Successful Applications: The results at temperatures of 316-386°C (600-727°F) and 25-450 kW/m² (55-990 BTU/hr-in²) indicated that the calculated thermal conductivity from the model was systematically lower than the measured values (error of ~25%).

Limitations: The selection of the geometry (for example, octahedral magnetite crystal contacts and the relative thickness of the layer with parallel arrangement of the plates) and the conducting media (steam, water or solid deposit) will have a significant impact on the result. Knowledge of the geometry of actual deposits may need to be improved in order to select these characteristics of the model. Actual deposits have the inactive layer near the heated surface and the active layer near the bulk fluid. The model described by the author has these layers reversed. This probably has minimal impact on the results because heat removal by active steaming within the deposit is not considered. Conclusions are made about the impact of wick boiling with minimal explanation. This may be sufficient since

conduction (not wick boiling) may be the principle heat transfer mechanism through deposits in supercritical boilers in regions where there is a high probability of boiler tube failure. An empirical coefficient is used.

Significant Application Observations: Within the limitations (cited above), the authors make the observations that (a) 0.2-0.3 mm (7.9-12 mils) deposits can result in dramatic increases in tube temperature.

Possible Refinements: This model could be combined with a steaming model.

Assessment for Fossil Plant Application: This model may apply to superheated region of boilers, but does not apply to boiling region. The strong dependence on regular patterns within the proposed model may limit its utility.

Output Parameter(s): Thermal Conductivity of Deposit for Ferrous Oxide Deposit with Water in Pores (0.5-1.4 and 1.3-2.5 W/m-°K or 0.1-1.0 and 1.0-1.9 BTU/hr-in-°F with boiling steam channels and without boiling steam channels, respectively)

Input Parameters:

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Temperature	None	316-386°C (601-727°F)	None	Calculations were Done Over a Range of 50–500°C (122-932°F)
Thermal Conductivity (Deposit Layers)	Ferrous Oxide Without Pores	6.9 W/m-°K (5.1 BTU/hr-in-°F)	Temperature	

2.2.2 Mass Transfer Equations and Models

2.2.2.1 Time Dependent, Mass Transfer

Deposition Mechanism: Insoluble Material

Source: Povarov and Petrova,⁽³⁾ Part 2 of 2

Description: This model was designed to predict the impact of mass transfer on deposition of insoluble material.

Assumptions: All effects of mass transfer can be described by a mass transfer coefficient. The coefficient accounts for two simultaneous processes (deposition and release of suspended impurities).

Results

Successful Applications: The equations have been tested at various pressures with cobalt and manganese oxide depositions.

Limitations: Data appear to have been collected from bench scale tests. Mass transfer coefficients are available only for cobalt and manganese oxides. Velocity effects are not considered in equations explicitly, i.e., velocity effects are shown in the graphs, but not in the equations. Mass transfer and heat flux equations are provided, but they are not connected to each other. A noted significant impact of enthalpy is not addressed in the equations.

Significant Application Observations: Large experimental data base.

Possible Refinements: None

Assessment for Fossil Plant Application: Data were collected for conditions similar to fossil plants.

Output Parameter(s): Deposit Rate for Solids ($0.5\text{--}3.5 \text{ mg/m}^2\text{-hr}$ or $7 \times 10^{-6}\text{--}5 \times 10^{-5} \text{ lbm/in}^2\text{-hr}$)

Input Parameters:

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Time	None	1–30 hours	None	Mass Transfer Coefficient Varies with Time (at Least in the First Few Hours)
Temperature	None	Up to 449°C (840°F)	None	Impacts Mass Transfer Coefficient
Pressure	None	31-248 kg/cm ² (30-240 at, 440-3,530 psi)	None	Impacts Mass Transfer Coefficient
Mass/Volume (Bulk)	None	Not Cited	None	None
Velocity	None	0.0005-0.001 m/s or 0.0016-0.0033 ft/s Near Wall and 0.3-3.0 m/s or 1-10 ft/s in Middle of Tube (Dependent on with Time Through 1.8 m/s or 5.9 ft/s)	None	Velocity Not Explicitly Included in Equations; Impacts Mass Transfer Coefficient

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Density (Water)	None	Consistent with Temperature and Pressure of Bulk Fluid	Temperature and Pressure	None
Surface Area (Deposit)	None	Not Cited	None	None
Mass Transfer Coefficient	Time, Temperature, Pressure and Velocity	Zero When Deposition Equals Release	None	None
Concentration (Bulk) of Depositing Material	None	100–400 ppb	None	Concentrations of Insoluble Cobalt and Manganese Oxides
Particle Size	None Cited	0.4 micron (0.016 mil)	None Cited	Parameter Not Included in Equation
Size and Composition of Substrate Tube	Stainless Steel	0.75 mm (30 mils)	None	Parameter Not Included in Equation
Oxygen	None	60–100 ppb	None	Parameter Not Included in Equation
pH	None	5.5–7.0	None	Parameter Not Included in Equation

2.2.2.2 Time Dependent, Diffusion and Electrophoresis

Deposition Mechanism: Insoluble Material

Source: Matijevic, *et al.*⁽⁷⁾

Description: This model was designed to describe deposition of metal oxide colloidal particles from liquid, aqueous dispersions onto stainless steel surfaces as a result of London-van der Waals forces and the Born (steric) repulsion. Data are presented on the impact of adjacent solution chemistry (ionic strength and pH). The rate of deposition and repulsion increases with increasing ionic strength until a threshold is reached beyond which increasing ionic strength does not change the equilibrium. The attraction decreases with increasing temperature (25°C or 77°F compared to a maximum of 210°C or 410°F). There is an exponential change in the particle number concentration as a function of total surface of substrate in contact with the liquid and the total volume of liquid. Detachment of particles is also exponential depending on the number of deposited particles and the volume of liquid

Results

(and possibly other factors that were not investigated. A correlation between (1) the product of electrophoretic mobility of hematite and steel as a function of pH and (2) the adhesion rate of hematite with the surface coverage of steel by hematite particles as a function of pH was shown to have the same trend. The deposition rate sharply decreases once saturation by adhered particles brings about charge reversal of the substrate.

Assumptions: Uniform particle shape is an integral part of the deposition process, according to the authors. Particles with diameters near 0.15 micron (0.006 mil) deposit in accordance with diffusion theory. Particles with diameters greater than 0.5 micron (0.008 mil) form deposits at a rate that is higher than expected from diffusion theory.

Successful Applications: The authors have developed extensive laboratory experience in synthesizing and testing particles with uniform size and shape.

Limitations: Heat transfer is not present. Velocity is constant. The experiments were conducted so as to minimize the impact of electrostatic attraction between the particles and the substrate by selection of particles and substrates of like charges. Selecting unlike charges could result in possible high bias in deposition rate. However, like charges can be repulsive, possibly resulting in low bias in deposition rate. While the paper discusses the influence of deposition of Fe_2O_3 (hematite) on steel in a packed bed, the argument revolves around experimental data only. Although a number of parameters that are used in the calculations (porosity, density of particles, flow rate, etc.) are not given explicitly in this reference, the principle author has published several hundred papers that may give more information. The apparatus appears to be similar to that described in Reference 9.

Significant Application Observations: The adhesion process can be interpreted in terms of the existing theories of interactions of unlike particles combined with the kinetics of particle diffusion. The deposition of colloidal particles on planar surfaces in the absence of shear is governed by convective diffusion, whereby the charges on the particles and the substrate play a dominant role.

Possible Refinements: None

Assessment for Fossil Plant Application: The equations and data may be useful, but they need to be extrapolated to higher temperature, pressure and heat flux.

Output Parameter(s): Mass Deposited

Input Parameters:

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Time	None	No range given	None	None
Temperature	None	22 and 210°C (72 and 410°F)		Temperature is Not Included in Equations

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Mass or Volume (Bulk)	None	No range given	None	None
Velocity	None	Laminar	None	Velocity Chosen to be Laminar So That Only Diffusion is Measured
Particle Size	β -FeOOH (Rod- like) Fe ₂ O ₃ (Spherical)	Diameter = 0.02 micron (0.0008 mil) and Length = 0.25 micron (0.0098 mil) Diameter = 0.15 micron (0.0059 mil) and 0.50 micron (0.020 mil)	None	None
Density (Particle)	None	Not Cited in this Reference	None	None
Mass Particles (Total)	None	Not Cited in this Reference	None	None
Surface Area (Substrate)	None	Not Cited in this Reference	None	None
Number Particles Deposited	None	Not Cited in this Reference	None	None
Porosity (Deposit)	None	Not Cited in this Reference	None	None
Diffusion Coefficient	None	Not Cited in this Reference	None	None
Concentration (Bulk) of Depositing Material	None	Not Cited in this Reference	None	None
Concentration of Contaminants	None	10 M NaNO ₃ 0.1 M Ca(NO ₃) ₂	None	This Parameter May Not be Included in Equations. The Electrolyte is Designed to Control Electrostatic Attraction and Repulsion

Results

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
pH	Results from Electrolyte Addition to the Suspension	3–8		This Parameter May Not be Included in Equations
Mass Transfer (Convection)	None	Not Cited in this Reference	None	None
Mass Transfer (Diffusion)	None	Not Cited in this Reference	None	None

2.2.2.3 Time Dependent, Mass Balance

Deposition Mechanism: Insoluble Material

Source: Beal and Chen⁽⁸⁾

Description: This model was designed to provide a mass balance for deposition, including turbulent deposition, boiling enhanced deposition, gravitational settling, sticking probability, re-entrainment and growth. Output is a function of particle size and the geometry of the deposition surface (horizontal or vertical). A region-to-region flow rate is used, and the results are obtained by iteration.

Assumptions: No distinction is made between various corrosion products (iron, nickel and copper) based on the assumption that the densities are similar.

Successful Applications: The model has been applied to a full-sized nuclear steam generator. However, benchmarking against actual steam generator deposits was suggested as a future activity.

Limitations: Some coefficients are calculated and some appear to be arbitrary. The model was designed for a nuclear steam generator and requires considerable knowledge of the internal thermal-hydraulic operation of various regions within the steam generator (economizer, boiling region, etc.). Only corrosion products are considered (dissolved material is not considered).

Significant Application Observations: There is a need for experimental data describing growth or behavior of deposits under some specific localized changes.

Possible Refinements: Combine with other available models.

Assessment for Fossil Plant Application: The report is extensive, and the author makes some significant contributions toward providing equations for various deposition processes and defining some coefficients that are difficult to determine from current information. This

model could provide some equations for the initial formation the deposits (prior to development of chimneys).

Output Parameter(s): Deposit Rate for Solids (1.5×10^{-2} – 9.1×10^{-5} g/cm² or 2.1×10^{-4} – 1.3×10^{-6} lbm/in² on Tubes, 9.3×10^{-4} – 210 g/cm² or 1.3×10^{-5} – 3.0 lbm/in² on Horizontal Tubesheet Surfaces at Bottom and 1.6×10^{-4} – 7×10^{-4} g/cm² or 2.3×10^{-6} – 9.9×10^{-6} lbm/in² on Horizontal Tube Supports) or 0-7 g/cm² or 0-9.9x10⁻² lbm/in²)

Input Parameters:

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Time	None	Several Years (1-5 Years in an Example)	None	Initial Transient Appeared to Require 0.5 Year to Reach Steady State
Flow Rate (Region-to-Region)	Total Feedwater Flow Rate = 1.04×10^6 kg/hr (4.74×10^5 lbm/hr)	0.2-100% of Total Feedwater Flow Rate	None	None
Temperature	None	278°C (532°F)	None	None
Deposit Mass	None	0.014-0.049 mg (3.0×10^{-8} – 1.1×10^{-7} lbm)	None	None
Velocity	None	0.15–3 m/s (0.5–10 ft/s)	None	Not Directly Used as Input Parameter
Particle Density	None	3 g/cm ³ (187 lbm/ft ³)	None	None
Density (Water)	None	0.76 g/cm ³ (47.2 lbm/ft ³)	Temperature and Pressure	None
Dynamic Viscosity	None	3.5 g/cm-hr (0.234 lbm/ft-hr)	None	None
Surface Area (Substrate)	None	0.24×10^8 cm ² (3.7×10^6 in ²)	Surface Smoothness	None
Particle Size	None	0.2-20 micron (0.008-0.8 mil)	None	None
Deposition Coefficient	Particle Size and Configuration (Horizontal or Vertical) of Deposition Surface	----	Schmidt Number, Viscosity, Friction Velocity, Wall Shear Stress, Fluid Density	None

Results

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Re-entrainment Coefficient	None	Calculated to be 0.023–0.0056/s	Wall Sheer Stress, Dynamic Viscosity, Particle Size and Fraction of Particle in Turbulent Region	Theory overpredicts experimental values by 10x
Re-entrainment Correlation Factor	None	1 for Thin Deposits and Higher for Thicker Deposits	None	None
Growth Rate Coefficient	None	Not Cited	Particle Size	No known method of calculation
Concentration (Bulk) of Depositing Material	None	730–1500 ppb	None	None
Blowdown Rate	None	22–47%	None	None

2.2.2.4 Steady State, Mass Transfer and Deposition

Deposition Mechanism: Insoluble – Solid Particle

Source: Kuo and Matijevic,⁽⁹⁾ Part 1 of 3

Description: Equation proposed to explain the interactions of uniform spherical hematite particles with stainless steel as a function of pH, flow rate, temperature and other chemicals (sodium dodecyl sulfate and ethylenediaminetetraacetic acid).

Assumptions: Uniform shape of particles is important in the deposition process.

Successful Applications: Results are based on bench-scale laboratory experiments using ferric oxide (hematite) on a stainless steel substrate.

Limitations: Input values for “sticking factor” may be difficult to define for all applications (or applications other than those for which data were collected). Data are limited to iron oxide deposition onto a stainless steel substrate at relatively low temperatures, i.e. below 80°C (176°F).

Significant Application Observations: Deposition occurred only over a narrow pH range. Deposition increased with decreasing velocity in the range of 0.01–0.1 cm/s (0.0003–0.003 ft/s).

Possible Refinements: Add constants for elevated temperature application of equation.

Assessment for Fossil Plant Application: Temperature of experiments may limit usefulness of available coefficients.

Output Parameter(s): Contact Efficiency (Dimensionless ratio of the rate of particles flowing toward collector and the rate of particles striking collector)

Input Parameters:

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Temperature	None	25-80°C (77-176°F)	None	Temperature is not included in equation
pH	Adjusted with sodium hydroxide and nitric acid	3–12	None	pH is not included in equations
Surface Area (Deposit Diameter)	None	9 mm (0.35 in)	None	Also referred to as deposit diameter
Porosity (Deposit)	None	38%	None	Also referred to as void fraction of deposit
Deposit Thickness	None	2.6 cm (1 in)	None	Column length in experiment
Sticking Factor	Material selection	0–1	Number of collisions that produce adhesion Total number of collisions	May be difficult to define
Concentration (Depositing Material in Bulk Fluid)	Concentration input and concentration output	Approx. 10^8 particles/cm ³	None	None

2.2.2.5 Steady State, Mass Transfer and Adhesion

Deposition Mechanism: Insoluble - Solid Particle

Source: Kuo and Matijevic,⁽⁹⁾ Part 2 of 3; uses relationship of Levich⁽¹⁰⁾

Description: An equation from Levich⁽¹⁰⁾ that models transport of particles onto a surface was tested with laboratory data of Kuo and Matijevic.

Assumptions: Attachment (adhesion) occurs as second step after transport to surface. Adhesion is governed by forces that depend on material composition. Transport is governed

Results

by diffusion, interception and gravity settling. Particles smaller than 1 micron (25.4 mils) are transported by diffusion.

Successful Applications: Results are based on bench-scale laboratory experiments and are fit to the equation of Levich.⁽¹⁰⁾

Limitations: Data are limited to iron oxide deposition onto a stainless steel substrate at relatively low temperatures, i.e. below 80°C (176°F). Velocity is lower than actual plant applications. The correlation is made in a range where no activation energy was required (near neutral pH).

Significant Application Observations: None

Possible Refinements: Combine with equation that includes concentration and confirm application for elevated temperatures.

Assessment for Fossil Plant Application: Temperature extrapolation is uncertain.

Output Parameter(s): Contact Efficiency (Dimensionless ratio of the rate of particles flowing toward collector and the rate of particles striking collector)

Input Parameters:

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Temperature	None	25-80°C (77-176°F)	None	None
Velocity	None	0.01–0.1 cm/s (0.0003-0.003 ft/s)	None	None
pH	Adjusted with sodium hydroxide and nitric acid	3–12 (correlation is done at 6 – 7)	None	pH is not included in equations
Viscosity (Liquid)	May be altered by concentrating of chemicals	$3.5\text{--}8.9 \times 10^{-3}$ p	None	None
Particle Size (Diameter)	None	0.17 micron (0.0067 mil)	None	Uniform particle size may need to be replaced with range of particle size for real systems

2.2.2.6 Steady State, Desorption

Deposition Mechanism: Insoluble - Solid Particle

Source: Kuo and Matijevic,⁽⁹⁾ Part 3 of 3

Description: Equations designed to predict desorption of particles from a metal surface.

Assumptions: Chemical interaction and densification were not considered to impact the removal of deposits from the substrate. These phenomena may significantly alter the result.

Successful Applications: Results are based on bench-scale laboratory experiments.

Limitations: Data are limited to iron oxide and chromium hydroxide release from a stainless steel substrate at relatively low temperatures, i.e. below 80°C (176°F). Velocity is lower than actual plant applications. One input parameter references earlier work that was not reviewed.

Significant Application Observations: Desorption did not change in the range of 0.03–0.13 cm/s (0.01–0.05 in/s).

Possible Refinements: None

Assessment for Fossil Plant Application: Although the equations and constants will be difficult to apply directly to practical systems, the equations may allow some insight into deposition mechanisms and energies.

Output Parameter(s): Interaction Potential Energy

Input Parameters:

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Temperature	None	25–80°C (77–176°F)	None	Although temperature is used in the equations, the results are plotted with temperature as a parameter in the output (energy/temperature)
Particle Size (Diameter)	None	0.25 micron (0.01 mil)	None	Uniform particle size may need to be replaced with range of particle size for real systems

Results

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Hamaker Constant (Overall)	This constant varies for differing materials systems and different temperatures	0.22–6.2 x 10^{20} J (2.0- 59×10^{-24} BTU)	None	Constant given only for small range of material systems and temperatures.
Dielectric Constant	Varies with liquid media	Not given	None	None
Surface Potential	Dependent on material composition	Not given	None	None
Unit Charge	None	Not given	None	None
Separation Distance	None	0–150 Angstroms (0- 5.9×10^{-7} in)	None	This distance is assumed over a predetermined range to allow calculation of the amount of interaction energy as a function of distance.

2.2.3 Solubility Equations and Models for Steam and Water

2.2.3.1 Steady State, Chemistry (Steam Model)

Deposition Mechanism: Soluble Material

Source: Leibovitz⁽¹¹⁾

Description: Equations designed to predict the solubility of chemicals in dry steam (vaporous carryover).

Assumptions: None

Successful Applications: Considers sodium hydroxide, sodium chloride, sodium sulfate, sodium hydrogen sulfate, hydrochloric acid, sulfuric acid and mixtures.

Limitations: This is a model that uses experimental data from other investigators to devise constants. Moisture carryover is not included.

Significant Application Observations: One sample calculation was performed to illustrate the model, but insufficient data were available for comparison at the time.

Possible Refinements: Compare to results of experimental data for steam solubility that has been collected since the model was prepared.

Assessment for Fossil Plant Application: Model appears to be applicable to fossil plants, but needs to be confirmed by comparison to experimental data

Output Parameter(s): Concentration of Chemical in Steam (ppm or ppb)

Input Parameters:

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Temperature	None	None given	None	Temperature is Fixed
Pressure	None	None given	None	Pressure is Input for Steam and Water Densities
Density (Steam)	None	None given	Temperature and Pressure	None
Density (Water)	None	None given	Temperature and Pressure	None
Concentration of Liquid Concentrate	Chemical composition	None given	Temperature and Pressure	None
Distribution Ratio	Chemical composition	None given	Temperature and Pressure	None
Dissociation Constant	Chemical composition	None given	Temperature and Pressure	None
Solubility Constant	Chemical composition	None given	Temperature and Pressure	None
Hydration Number for Associated Species	Chemical composition	0.5–10	Temperature and Pressure	None
Hydration Number for Dissociated Species	Chemical composition	None given	Temperature and Pressure	None

2.2.3.2 Steady State, Chemistry (Steam Testing and Equations)

Deposition Mechanism: Soluble Material

Source: Allmon, *et al.*^(12,13)

Description: Equations designed to predict the solubility of chemicals in dry steam (vaporous carryover).

Assumptions: Assumes maximum concentration in liquid deposit predicted by thermodynamic equilibrium considerations. Equations do not consider possible impact of

Results

system dynamics, although considerable discussion is presented on possible impact of kinetics.

Successful Applications: Results are based on bench-scale and pilot-scale experiments with sodium hydroxide, sodium chloride, ammonium chloride, ammonium sulfate and corrosion products (iron, nickel and chromium).

Limitations: Only data available for sodium hydroxide is sufficient for development of correlating equations. Moisture carryover is not included.

Significant Application Observations: Hydrolysis (reaction with water) was observed to result in multiple chemical species that may transport in steam at different rates (for example, sodium chloride produces sodium hydroxide and hydrochloric acid). Metal (iron, etc) solubility enhanced significantly in presence of chemical additives.

Possible Refinements: These data/equations may be combined with those of other investigators.

Assessment for Fossil Plant Application: These results should be considered in conjunction with more recent data.

Output Parameter(s): Concentration of Chemical in Steam (ppb or ppm)

Input Parameters:

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Temperature	None	Maximum of 130–345°C (266–653°F)	None	Experiments cover broader range (lower temperatures)
Pressure	None	49 kg/cm ² (4.8 MPa, 700 psi)	None	Experiments conducted up to 6.9 MPa (1000 psi)
Steam Density	None	Up to 0.019 g/cm ³ (1.2 lbm/ft ³)	Temperature and Pressure	Consistent with temperature and pressure
Concentration of Liquid Concentrate	Chemical Composition	0–100%	Temperature and Pressure	Consistent with temperature and pressure
Distribution Ratio	Chemical Composition	0.1–40x10 ⁻⁸	Temperature and Pressure	None

2.2.3.3 Steady State, Chemistry (Steam Testing)

Deposition Mechanism: Soluble Material

Source: Rogers⁽¹⁴⁾

Description: Equations designed to predict the solubility of chemicals in dry steam (vaporous carryover).

Assumptions: Assumes maximum concentration in liquid deposit is predicted by thermodynamic equilibrium considerations.

Successful Applications: Results are based on bench-scale experiments.

Limitations: Data available for only sodium chloride and sodium sulfate at one temperature. Although an equation is provided, the constants must be obtained from a graph. Hydration of sodium chloride and sodium sulfate complicates the interpretation of results. Moisture carryover is not included.

Significant Application Observations: Hydrolysis (reaction with water) was observed to result in multiple chemical species that may transport in steam at different rates (for example, sodium chloride produces sodium hydroxide and hydrochloric acid).

Possible Refinements: These data/equations may be combined with those of other investigators.

Assessment for Fossil Plant Application: These results should be considered in conjunction with more recent data.

Output Parameter(s): Concentration of Chemical in Steam (ppm or ppb)

Input Parameters:

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Temperature	None	Maximum of 300–550°C (572–1022°F)	None	None
Pressure	None	62–106 kg/cm ² (6.0–10.3 MPa)	None	None
Hydration Number for Associated Species	Depends on chemical	0.18–3.66 for NaCl	Depends on partial molar volume (reciprocal density) of steam	Calculated from literature

Results

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Steam Density	None	4.2–39 g/L (0.26–2.4 lbm/ft ³)	Temperature and Pressure	Also referred to as partial molar volume
Correlation Constants	None	Not given directly	None	None

2.2.3.4 Time Dependent, Chemistry (Hideout And Hideout Return)

Deposition Mechanism: Soluble Material

Source: Mann and Castle⁽¹⁵⁾

Description: The author provides models for Hideout (HO) and Hideout Return (HOR) of chemicals in nuclear steam generators crevices plus an assessment of similar models proposed by other investigators. Experiments were conducted at various heat flux, superheat and bulk concentrations for hideout and hideout return.

Assumptions: Equilibrium (final) mass of salt is known for hideout. If this value is not known or cannot be determined, the equations would need to be rearranged to account for geometry of the capillaries and chimneys.

Successful Applications: The author applies hideout model to experimental results for a flow into a crevice with known geometry. The test fixture formed a crevice that was packed with carbon fibers. Heat flux was from a nickel-plated Alloy 600 tube into the crevice. The crevice was bounded by a Type 1018 carbon steel support that surrounded the tube. Both the top and the bottom of the crevice were open (not welded). Chemical were fed into an autoclave that contained the test fixture and were concentrated in the crevice by the heat flux. An excellent correlation was shown between the experimental results and the model predictions. The equilibrium mass of salt in a crevice was found at a high concentration of salt (12 ppm sodium chloride) in the bulk fluid in an autoclave with an appropriate heat flux (125 kW/m² or 275 BTU/hr-in²). The equilibrium mass was the amount above which additional exposure time resulted in no additional uptake by the crevice. Then, the hideout (HO) model was applied to lower concentrations (down to 12 ppb) successfully. The author also studied hideout return (HOR) and applied diffusion equations to the HOR data. Unfortunately, the geometric parameters needed for the diffusion equation were not known for the HOR. Therefore, the author used the time constant from the HOR data to calculate the geometric parameters.

Limitations: The HO model does not predict the final (equilibrium mass) of the salt in a deposit; the model predicts the rate of salt uptake prior to reaching equilibrium. If the geometry is unknown or the equilibrium mass cannot be measured experimentally, the model cannot be solved. Likewise, the HOR model cannot be used to calculate the HOR time constant without knowledge of the geometry of the deposits.

Significant Application Observations: The rate of hideout was reduced significantly in a corroded crevice, possibly as a result of changes in the porosity of the crevice as a result of accumulation of iron oxides in the crevice. This condition may result in a reduction in the rate of evaporation and produce steam blanketing. The effective diffusion coefficient is a function of porosity and tortuosity. According to this reference permeability is proportional to porosity raised to a power between 5.5 and 12, depending on deposit morphology. The higher value is close to that found for various power station sludge deposits. The calculated lithologic factor (length of steam chimney divided by thickness of deposit) for corrosion grown magnetite was 14.

Possible Refinements: None

Assessment for Fossil Plant Application: The HO and HOR models may be applicable to fossil boiler deposits, but a method for estimation of the equilibrium mass or deposit geometry would be needed.

Output Parameter(s): Hideout: Mass of Salt Deposited ($0.01\text{-}14\text{ mg}$, $2.2 \times 10^{-8}\text{--}3.1 \times 10^{-5}\text{ lbm}$ or $0.02\text{-}9\text{ ppm Cl}$) and Concentration Factor ($2 \times 10^3\text{--}7 \times 10^5$); Hideout Return: Lithologic Factor

Input Parameters for HO:

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Time	None	0.9-64.8 hr	None	None
Heat Flux	None	Approx. 50-300 kW/m ² (110-660 BTU/hr-in ²)	None	HO Tests Were Conducted at Constant Heat Flux
Superheat	None	0-102°C (0-180°F)	None	None
Crevice Gap	None	0.23-0.3 mm (9.1-12 mils)	None	None
Mass/Volume (Bulk)	None	Not Cited	None	Autoclave
Heat of Vaporization	None	Not Cited	None	Use Handbook Value
Porosity	None	50%	None	Initial Value with Carbon Fiber. Does not Include Corrosion Product (Formed in Place) This Parameter is Not Used in Equations

Results

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Pressure	None	65 kg/cm ² (64 Bar, 930 psi)	None	This Parameter is Not Used in Equations
Temperature (Bulk)	None	280°C (536°F)	None	This Parameter is Not Used in Equations
Flow Rate	None	2.2 L/hr (0.0097 gal/min)	None	Autoclave Bulk Flow Rate This Parameter is Not Used in Equations
Concentration (Bulk) of Depositing Material	Sodium Chloride	12 ppb – 12 ppm	None	Also Tested Ammonium Chloride (0.07-3.5 ppm Cl to Corrode the Crevice)

Input Parameters for HOR:

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Time	None	16-66 Hours	None	None
Time Constant	Geometry Specific	30-180 Minutes (Calculated) 50 Minutes (Experimental)	Length of Crevice Effective Diffusion Coefficient	Time for Concentration to Decay in Half
Concentration of Depositing Material	Sodium Chloride	Not Cited Explicitly	None	Used to Calculated Time Constant
Superheat	None	45°C (81°F)	None	None
Porosity (Deposit)	None	22-51%	None	None
Length of Crevice Not Filled with Concentrate	None	Not Known	None	None
Total Chimney Length	None	0.2-0.3 mm (8-12 mils)	None	None
Tortuosity	None	1-2.6	None	None
Diffusion Coefficient	None	Not Cited	Porosity Tortuosity	None

2.2.3.5 Time Dependent, Chemistry

Deposition Mechanism: Insoluble Material

Source: Voronov and Krasnoryadtsev⁽¹⁶⁾

Description: This model was designed to consider the change of iron deposits through the use of chelating agents during plant operation. It is a combination of mass balance for insoluble and soluble substances. Soluble materials are treated through (a) changes of concentration of chelated solution through decomposition, (b) specific fouling of heat transfer surfaces, (c) iron in chelated and unchelated form in the deposits and (d) flow rates of steam, feedwater and blowdown. Connection is made between concentrations of chelating agents and change of fouling of heat exchange surfaces.

Assumptions: The steam generator can be described for this application by dividing the steam generator into 80 sections. A set of differential equations is needed for each section to describe the kinetics of the processes. Discharge from one section is the input to the next section.

Successful Applications: Although it was applied to a Russian fossil steam generator (PGV-1000), the results of the application are not presented. Some plant information is presented.

Limitations: A large number of conversion factors are required, including the proportion of friable layer of deposits, proportion of chelate and iron in unchelated form in steam, rate of thermal decomposition of chelate and specific fouling of a given surface. Incomplete information is presented.

Significant Application Observations: None

Possible Refinements: None

Assessment for Fossil Plant Application: The equations may have some application, but the lack of specific parameters makes practical use difficult.

Output Parameter(s): Removal Rate for Solids (Quantity of Chelated Iron Exchanged Between Sections, $0-0.4 \times 10^{-1}$ ppm-s)

Input Parameters:

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Time	None	Not Cited	None	None
Heat Flux	None	Not Cited	None	None
Mass/Volume (Bulk)	None	Not Cited	None	None

Results

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Flow Rate	None	Not Cited	None	None
Deposit Surface Area	None	Not Cited	None	None
Deposition Rate	None	Not Cited	None	None
Re-entrainment Coefficient	None	Not Cited	None	None
Concentration of Contaminants In Bulk Liquid	None	10 ppb Na	None	None
Concentration Factor Between Sections	None	10–320x	None	This Parameter May Not Be Used in Equations
Concentration of Depositing Material in Bulk Liquid	None	Not Cited	None	None
Density of Concentrated Liquid	None	Not Cited	None	None
Blowdown Rate	None	Not Cited	None	None
Concentration in Steam	None	Not Cited	None	None

2.2.4 Particle (Corrosion Product) Equations and Models

2.2.4.1 Time Dependent, Chemistry – Deposition and Corrosion

Deposition Mechanism: Insoluble Material

Source: Liebovitz⁽¹⁷⁾

Description: This model was designed primarily to model corrosion in crevices, but also includes some deposition equations. This model also contains some ion exchange properties for magnetite.

Assumptions: Pores are approximated by straight channels perpendicular to the surface. Transport is one dimensional along these channels by electromigration and/or diffusion. Concentration may vary along the length of the channel, and consequently, magnetite may precipitate. Porosity may change as corrosion progresses. Quasi steady-state conditions may apply; processes are irreversible.

Successful Applications: See below.

Limitations: The model primarily addresses corrosion of carbon steel. The output has two dependent variables (one of the independent variables is insufficiently described by the equations).

Significant Application Observations: The model was compared to available capsule test data for carbon steel in various combinations of sea salt, sodium hydroxide, copper chloride, nickel chloride, sodium chloride and boron. The model over predicted the corrosion rates by 100x.

Possible Refinements: May provide an alternative diffusion term that includes corrosion.

Assessment for Fossil Plant Application: Model equations may be useful on first principle basis. However, the tendency to significantly over predict corrosion would need further consideration.

Output Parameter(s): Deposit Thickness (microns/mils or microns per month/mils per month) and One of the Input Parameters; Concentration Factor (100-7500x)

Input Parameters:

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Time	None	0-400 days	None	None
Porosity (Deposit)	None	20-40%	None	None
pH	None	2-9	None	None
Concentration (Bulk) of Depositing Material	Iron	None	None	Iron Concentration Originates from Corrosion Processes (Not from Bulk Solution)
Concentration (Bulk) of Contaminants	Chloride	0.1-100 ppm	None	Neutral Chloride Salt Effect on Corrosion
Current Density (Corrosion)	None	0.8-400 micro-amperes/cm ² (5.2-258 micro-amperes/in ²)	Voltage = 0-5 mV	None

2.2.5 Mixed Models

2.2.5.1 Time Dependent, Continuity, Momentum, Energy and Heat Transfer, Including Local Fluid Dynamics

Deposition Mechanism: Soluble Material

Source: Jones, *et al.*^(18,19)

Description: A vapor bubble model describes the initial accumulation of deposits leading to the capillaries and steam chimneys, and a deposit model refers to fully developed oxide deposits with capillaries and steam chimneys. The bubble model describes a vapor bubble, sitting on top of a heated surface, exchanging heat and mass with an infinite volume of subcooled water. This model solves simultaneously the momentum and energy equations. Field flow, concentration field and temperature field are decoupled for the vapor bubble. A deposit model was designed to predict the fluid dynamics and concentrating of chemicals in porous deposits and includes:

- (1) Darcy and continuity equations for pressure and flow distribution in a porous shell,
- (2) Equations for energy or heat transfer in a porous shell,
- (3) Schrage model for water flux at a chimney wall,
- (4) A diffusion equation for transport of solutes in a porous shell,
- (5) Yuan and Finkelstein equation for laminar pipe flow with uniform injection and suction to evaluate the pressure drop in a steam chimney and
- (6) Dry-out heat flux for a given deposit structure or the dry-out thickness for a given structure through a heat pipe wicking limit equation.

A relationship is provided to calculate the number of steam chimneys per unit area (chimney population) as a function of heat flux. Further, transport mechanisms in the deposit layer are described for molecular diffusion and mass convection of gaseous, molecular hydrogen and molecular oxygen. Only the diffusion equations are used in cylindrical coordinates. Deposition (exponential change in concentration) is a function of total surface of substrate in contact with liquid and the volume of passing liquid. Detachment of particles is also exponential depending on the number of deposited particles and the volume of liquid.

Assumptions: Bubble shape and volume are assumed to be constant with spherical symmetry. Heat transfer to the vapor bubble is considered negligible (zero thermal conductivity for vapor). The surrounding liquid is infinite in volume. Transient thermal capillarity due to thermal gradients is the only element in development of a vapor bubble. Mass transfer is considered only across the bubble surface. Porous structure surrounding a

chimney is isotropic and non-deformable. Water is non-compressible. Effects of gravity are negligible. Inertial effects are neglected.

Successful Applications: The model has been used to describe Axial Offset Anomaly (AOA) on fuel rods in nuclear power plants. The boron holdup in the deposit on the surface of the fuel is similar to the amount required for AOA based on estimates from neutronic calculations.

Limitations: The bubble and deposit models have not been combined. Currently, the bubble model does not consider the bubble growth in time, whereas the deposit model is time-dependent. The model could be combined with a fixed bubble size approach. Both models were developed for nuclear plant applications. The temperatures and pressures are lower than fossil boilers; however, the heat flux is similar to fossil boilers.

Significant Application Observations: A connection is presented between heating of a bubble, and its size increase, to the solute concentration increase at the intersection of the heating wall and bubble interface. A lower diffusion coefficient in the bulk gives rise to a higher maximum concentration value. Higher heat flux gives rise to a higher maximum concentration. Holdup of soluble material (boron) in a deposit was found to remain relatively low (near zero) until the deposit thickness reached a threshold (about 50 microns or 2 mils in the example presented by the authors).

Possible Refinements: Introduce variable volume for bubble to model bubble growth over time.

Assessment for Fossil Plant Application: This model may be applicable to concentrating of soluble material (corrodants and soluble metals) in fully developed deposits inside boiler tubes. The model may describe the consolidation (or densification) of deposits.

Output Parameter(s): (a) Concentration in Steam, (b) Concentration in Porous Medium, (c) Capillary Pressure, (d) Capillary Flow Field, (e) Capillary Temperature, (f) Pressure Drop in Steam Chimney, (g) Dryout Heat Flux (Wicking Limit, 15-190 W/cm² or 33-418 BTU/hr-in²), (h) Surface Temperature (Maximum of 44°C or 79°F Greater Than Bulk Temperature) And (i) Precipitated Deposit Thickness (Active Region of Precipitation (2-10 micron or 0.08-0.4 mil)

Input Parameters:

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Time	Bubble	1 s	None	Lifetime of bubbles is in milliseconds
	Deposit	Up to 196 Days		
Particle Size	Deposit	0.1-0.9 micron (0.004-0.035 mil)	None	None

Results

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Bubble Size	Bubble	5-10 micron (0.2-0.39 mil)	None	3,000-6,000 Bubbles/mm ² (2-4x10 ⁶ Bubbles/in ²)
Heat Flux	Bubble	100 W/cm ² (220 BTU/hr-in ²)	None	None
	Deposit	30-160 W/cm ² (66-352 BTU/hr-in ²)		
Temperature	Bubble	300-320°C (572-608°F)	None	None
	Deposit	345°C (653°F)		
Surface Temperature	Bubble	Not Given	None	None
	Deposit	44°C (79°F) Greater Than Bulk Temperature		
Subcooled Boiling	Bubble	None	None	None
	Deposit	10-35°C (18-63°F) Superheat		
Pressure	None	160 kg/cm ² (2250 psi)	None	None
Velocity	Bubble	None	None	Calculate Using Darcy Equation for Capillary Flow (1 micron or 0.04 mil))
	Deposit	2 x 10 ⁻³ m/s (6.6x10 ⁻³ ft/s at 150 bar (2,175 psi), T _{sat} , 100 W/cm ² (220 BTU/hr-in ²)		
Viscosity (Liquid)	Bubble	9.07x10 ⁻⁵ N-s/m ² (1.9x10 ⁻⁴ lbf-s/ft ²)	None	None
	Deposit	6.78 x 10 ⁻⁵ kgf-s/m ² (1.4x10 ⁻⁵ lbf-s/ft ²)		
Viscosity (Steam)	Bubble	Not Given	None	None
	Deposit	2.30x10 ⁻⁵ kgf-s/m ² (4.7x10 ⁻⁶ lbf-s/ft ²)		
Density (Water)	Bubble	713 kg/m ³ (44.5 lbm/ft ³)	None	None
	Deposit	592 kg/m ³ (37.0 lbm/ft ³)		

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Density (Steam)	Bubble Deposit	None 99.4 kg/m ³ (6.20 lbm/ft ³)	None	None
Specific Heat	Bubble	5.79x10 ³ J/kg-K (1.38 BTU/lbm-°F)	None	None
Heat of Vaporization	Bubble Deposit	1.404x10 ⁶ J/kg (6.035x10 ² BTU/lbm) 9.67x10 ⁵ J/kg (4.16x10 ² BTU/lbm)	None	None
Diffusion Coefficient	Bubble Deposit	0.37-7.7x10 ⁻⁹ m ² /s (3.9-82.9x10 ⁻⁹ ft ² /s) 1.27x10 ⁻⁸ m ² /s (1.37x10 ⁻⁷ ft ² /s)	Bubble Given for LiOH in Water at 100°C (212°F) Diffusion Coefficient of Solute in Porous Shell	Equations Given to Relate Diffusion Coefficient to Electrical Conductivity
Surface Tension	Bubble Deposit	2.3x10 ⁻⁴ N/m-K (1.3x10 ⁻⁶ lbf/in-K) 4.56x10 ⁻³ N/m (2.6x10 ⁻⁵ lb/in)	Temperature	None
Thermal Diffusivity	Bubble	1.37x10 ⁻⁷ m ² /s (1.47x10 ⁻⁶ ft ² /s)	None	None
Concentration of Contaminants in Bulk Liquid	Bubble Deposit	2 ppm Li 0-5 ppb Cu (as CuO), 900 ppm B (as Boric Acid) and 2ppm LiOH	None	None
Interfacial Heat Transfer Coefficient	Bubble Deposit	2.7x10 ⁷ W/m ² -K (4.7x10 ⁶ BTU/ft ² - hr-°F) 5.53x10 ⁶ W/m ² -K (9.7x10 ⁵ BTU/ft ² - hr-°F)	None	At Bubble Interface At Chimney Wall
Thermal Conductivity (Deposit)	Bubble Deposit	0.541 W/m-K (31.3 BTU/ft-hr- °F) 1.03 W/m-K (59.5 BTU/ft-hr-°F)	None	None

Results

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Deposit Composition	Bubble Deposit	None Nickel Ferrite (NiFe_2O_4), Nickel Oxide (NiO), Zirconium Oxide (ZrO_2), Nickel Iron Oxyborate (Bonaccordite, $\text{Ni}_2\text{FeO}_2(\text{BO}_3)$)	None	None
Chimney Radius	Bubble Deposit	None 2.5 micron (0.098 mil)	None	None
Chimney Population	Bubble Deposit	None $2,400\text{-}8,000/\text{mm}^2$ $1.5\text{-}5.2 \times 10^6/\text{in}^2$	None	Can be Measured Directly or Calculated from Heat Flux (Base Case $3,000/\text{mm}^2$ or $1.9 \times 10^6/\text{in}^2$ for Deposit)
Porosity (Deposit)	Bubble Deposit	None 30-80%	None	None
Capillary Cross- Sectional Area	Bubble Deposit	None Radius of Capillary = 1 micron (0.04 mil)	None	None
Fraction of Non-Chimney Surface Area	Bubble Deposit	None Calculate from Radius and Population	None	None
Total Chimney Length	Bubble Deposit	None Equal to Deposit Thickness	None	Active Deposition Thickness for Soluble Material 2- 10 micron (0.08-0.4 mil)
Deposit Thickness	Bubble Deposit	None 10-100 micron (0.4-4 mil)	None	None

2.2.5.2 Steady State, Permeability of Deposit Chimneys (Blake-Kozney Equation)

Deposition Mechanism: Soluble Material

Source: Eckert, *et al.*,⁽²⁰⁾ Part 1 of 2

Description: This equation was designed to calculate the permeability of the chimney portion of deposits based on physical characteristics of the deposits (porosity and particle size). Visualization studies and temperature measurements were made in a granular bed of nickel or copper particles as a contribution to the understanding of local dryout on the outside of two concentric glass tubes or between a square array of tubes. Additionally, tests were performed with a granular bed surrounding an array of tubes to study the height of the dryout region in the bed.

Assumptions: Three layers were considered in the analysis: (1) capillary, (2) chimney and (3) dryout. The equations herein describe the chimney region.

Successful Applications: None

Limitations: Deposit was heated from the sides and, as such, the boiling chimneys were parallel to the heat source. Conversely, heating in boiler tubes would be primarily from the base of the deposit (heating surface perpendicular to the boiling chimneys). Also, the equations are based primarily on the results of the lower temperature and lower heat flux tests in concentric glass tubes.

Significant Application Observations: Height of the wetted region is determined by the character of the bed (deposit) and by the boiling process. A dryout region occurs below the wetted region when the total height of the bed (deposit thickness) exceeds the height of the wetted region.

Possible Refinements: None

Assessment for Fossil Plant Application: Formula is a classic permeability equation, but the experiments were not successful.

Output Parameter(s): Deposit Permeability

Results

Input Parameters:

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Particle Size (Diameter)	Nickel Copper	Ni: Mean Diameter 28.3 micron (1.1 mils) Cu: Mean Diameter 17.3 micron (0.7 mils)	None	None
Porosity (Deposit)	Nickel Copper	65% 39%	None	None
Deposit Thickness	None	5.1, 10.2 and 15.2 cm (2, 4 and 6 in)	None	Column length in experiment Not an input parameter to the equations
Deposit Width	Concentric Tube Tube Array (Square)None	0.42 and 1.02 cm (0.16 and 0.4 in) 2.87 cm (1.13 in)	None	Gap between concentric or adjacent tubes in experiment Not an input parameter to the equations
Heat Flux	Concentric Tube Tube Array (Square)	Up to 1.3 kW/m ² (412 BTU/hr-ft ²) Up to 50 kW/m ² (10 ⁴ BTU/hr-ft ²)	Calculated from thermal resistance of tube and temperature difference	Not an input parameter to the equations
Temperature	Concentric Tube Tube Array (Square)None	120°C (248°F) 200°C (392°F)	None	Not an input parameter to the equations
Pressure	Concentric Tube Tube Array (Square)None	1 kg/cm ² (14.7 psia) 5.1 kg/cm ² (73 psia)	None	Not an input parameter to the equations

2.2.5.3 Steady State, Momentum, Continuity and Energy

Deposition Mechanism: Soluble Material

Source: Eckert, *et al.*,⁽²⁰⁾ Part 2 of 2

Description: This model was designed to calculate the length of the capillary or the length of the steam chimney as a function of heat flux, chimney radius, tortuosity, particle size and other parameters. The calculation starts with knowing the heat flux and either the capillary or chimney length and computes the other length.

Assumptions: Values were assumed for input parameters in the model.

Successful Applications: The theory behind the model is valid. Steam chimneys were visible in a few experiments, but were larger than actual steam chimneys in plant deposits.

Limitations: The analytical model is only loosely connected with the experimental results.

Significant Application Observations: None

Possible Refinements: None

Assessment for Fossil Plant Application: The length of the capillary may be calculated with these equations if other physical characteristics of the deposit and heat flux are known.

Output Parameter(s): Length of Steam Chimney or Length of Capillary

Input Parameters:

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Heat Flux	Concentric Tube	Up to 1.3 kW/m ² (412 BTU/hr-ft ²)	None	Selected Model Input Range
	Tube Array (Square)	Up to 50 kW/m ² (10 ⁴ BTU/hr-ft ²)		
Density (Steam)	None	0.5977 kg/m ³ (3.72x10 ⁻² lbm/ft ³)	None	Selected Model Input Value Values for Steam Chimney and Capillary (Start with Bulk)

Results

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Density (Liquid)	None	958.3 kg/m ³ (59.8x10 ⁻² lbm/ft ³)	None	Selected Model Input Value Values for Steam Chimney and Capillary (Start with Bulk)
Radius of Steam Chimney	None	1-10 micron (0.04-0.4 mil)	None	Selected Model Input Value
Population of Steam Chimney	None	Not Cited	None	Selected Model Input Value
Heat of Vaporization	None	2.58x10 ⁶ J/kg (11.1x10 ² BTU/lbm)	None	Selected Model Input Value
Radius of Capillary	None	0.1-1 mm (100-1000 micron or 4- 39 mil)	None	Selected Model Input Value
Viscosity (Liquid)	None	Not Cited	None	None
Porosity	None	65%	None	Selected Model Input Value
Steam Quality	None	Not Cited	None	None
Tortuosity	None	Not Cited	None	None
Permeability (Single Phase)	None	Not Cited	Radius of Capillary Population of Capillaries Tortuosity	None
Length of Deposit (Area Covered)	None		None	None
Surface Tension	None	0.0589 kg/s ² (0.12 lbm/s ²)	None	Selected Model Input Value

2.2.5.4 Time Dependent, Mass Transfer - Diffusion

Deposition Mechanism: Soluble Material

Source: Cleary, *et al.*,⁽⁵⁾ Part 1 of 5

Description: This model was designed to evaluate hideout and concentrating of soluble corrodants from the bulk water to and from crevices in nuclear steam generators. The work included estimation of diffusion coefficients for electrolytes in hot water, an experimental study of diffusion rates through simulated crevice packing, a study of contaminant hideout (HO) rates as a function of heat flux and a study of hideout return (HOR). Calculations of diffusion coefficients are reported for sodium chloride, hydrochloric acid in sodium chloride, divalent metal chlorides and two sodium-to-phosphate molar ratios at temperatures from 25°C (77°F) to greater than 300°C (572°F).

Assumptions: Diffusion coefficients for unobstructed liquid phase can be applied to crevices with inaccuracies of a few percent to approximately 40%, according to the authors.

Successful Applications: The mathematical model successfully described the hideout and hideout return in a laboratory test apparatus.

Limitations: Diffusion coefficients for obstructed porous deposits may vary by one order of magnitude from those estimated for this application, according to the authors. The calculated lithologic factor (essentially the ratio of effective diffusion coefficient in a crevice divided by the diffusion coefficient in the bulk fluid) is 2,100 at approximately 300°C (572°F) and about 200 at 20-90°C (68-194°F). The authors indicated that the low value for the lower temperatures may have resulted from “peripheral separation of the samples during cooling and preparation of capsule crevice-grown magnetite of the experiments.”⁽⁵⁾ Although convection mass transfer is included in the model and was calculated by the authors for input to the HO and HOR result, the authors did not assess convection mass transfer with the same rigor that was used for diffusion mass transfer and HO/HOR.

Significant Application Observations: At higher temperatures, it may be possible to use the diffusion coefficients for sodium chloride solutions as approximations for a variety of other monovalent electrolytes for which there are no data. Diffusion of dissolved ionic species through mechanically packed porous magnetite does not adequately simulate diffusion occurring through in-situ grown porous magnetite (2-5x smaller for packed magnetite).

Possible Refinements: None

Assessment for Fossil Plant Application: The equations should be applicable. Extension to higher temperatures would need to be evaluated.

Output Parameter(s): Mass Transfer Coefficient, Diffusion

Results

Input Parameters:

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Time	Cleary, <i>et al.</i>	Experimental Testing up to 600 Hours	None	None
Temperature	Other Cited Investigators Cleary, <i>et al.</i>	25-300°C (77- 572°F) Up to 100°C (212°F)	None	May Not Be Used Directly in Equations Crevice Superheat was 2-6°C (4-11°F) Wall-to-Crevice 7-12°C (13-22°F)
Pressure	Other Cited Investigators Cleary, <i>et al.</i>	Approx. 300 kg/cm ² (30 MPa, Approx 4,300 psi) Approx 1 kg/cm ² (Approx 1 atm, Approx. 15 psi)	None	May Not Be Used Directly in Equations
Cross- Sectional Area (Capillary)	Other Cited Investigators Cleary, <i>et al.</i>	Not Given 0.69 cm ² (0.11 in ²)	None	Not Certain that Crevice Cross- Sectional Area is Same As Chimney Cross- Sectional Area
Relative Viscosity	Sodium Chloride from Other Cited Investigators	1.1-1.7	Temperature (25- 300°C or 77- 572°F) and Concentration of 3.5-7 molal	May Not Be Used Directly in Equations
Length (Capillary)	Other Cited Investigators Cleary, <i>et al.</i>	Not Given 1.27 cm (0.5 in)	None	None
Diffusion Coefficient	Sodium Chloride from Other Cited Investigators	1.6-25.8 cm ² /s (1.7x10 ⁻³ -2.8x10 ⁻² ft ² /s)	Temperature (25- 300°C or 77- 572°F)	Bulk Fluid Diffusion is a Function of Ionic Mobility and Conductivity
Density (Concentrated Liquid)	Sodium Chloride from Other Cited Investigators	Not Given	None	None
Porosity	Cleary, <i>et al.</i>	25-38% (3-50% Through a Cross- Section of the Deposit)	None	May Not Be Used Directly in Equations

2.2.5.5 Time Dependent, Mass Transfer - Diffusion

Deposition Mechanism: Soluble Material**Source:** Cleary, *et al.*,⁽⁵⁾ Part 2 of 5**Output Parameter(s):** Mass Transfer, Diffusion (4.6×10^{-7} kg/hr)**Input Parameters:**

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Time	None	12–16 Weeks with Changes in Test Conditions Every 0.5–2 Days	None	Test Assemblies Removed Approx. Every 2 Weeks.
Flow Rate	None	42 L/day (11 gal/day)	None	Liquid Volume of Test Apparatus Exchanged Every 45 min
Mass Transfer Coefficient	None	Calculated from Above	None	None
Concentration (Bulk) of Depositing Material	Chloride (from Copper Chloride)	1-10 ppm	None	None
Concentration (Concentrated Liquid)	Chloride (form Copper Chloride)	1000 Times Bulk Concentration	None	None
Blowdown Rate	None	10%	None	None

2.2.5.6 Time Dependent, Mass Transfer - Convection

Deposition Mechanism: SOLUBLE MATERIAL**Source:** Cleary, *et al.*,⁽⁵⁾ Part 3 of 5**Output Parameter(s):** Mass Transfer, Convection

Results

Input Parameters:

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Time	None	12–16 Weeks with Changes in Test Conditions Every 0.5–2 Days	None	Test Assemblies Removed Approx. Every 2 Weeks.
Heat Flux	None	80-90 kW/m ² (176-198 BTU/hr-in ²)	None	None
Heat of Vaporization	None	Assume that of Water	None	None
Length, Wetted Chimney	None	46% of Total Length	None	None
Length, Total Chimney	None	1.27 cm (0.5 in)	None	None
Cross-Sectional Area, Chimney	None	0.69 cm ² (0.11 in ²)	None	Not Certain that Crevice Cross-Sectional Area is Same As Chimney Cross-Sectional Area
Concentration (Bulk) of Depositing Material	Chloride (from Copper Chloride)	1-10 ppm	None	None
Concentration (Steam)	None	Calculate from Other Investigators	None	None
Distribution Ratio (Steam/Water Concentration)	None	Obtain from Other Investigators	None	None
Activity Coefficient	None	Obtain from Other Investigators	None	None

2.2.5.7 Time Dependent, Chemistry - Hideout

Deposition Mechanism: Soluble Material**Source:** Cleary, *et al.*,⁽⁵⁾ Part 4 of 5**Output Parameter(s):** Hideout (450-470 mg, 9.9-10x10⁻⁴ lbm)

Input Parameters:

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Time	None	12–16 Weeks with Changes in Test Conditions Every 0.5–2 Days	None	Test Assemblies Removed Approx. Every 2 Weeks.
Heat Flux	None	80-90 kW/m ² (176-198 BTU/hr-in ²)	None	None
Heat of Vaporization	None	Assume that of Water	None	
Length, Wetted Chimney	None	46% of Total Length	None	None
Length, Total Chimney	None	1.27 cm (0.5 in)	None	None
Cross-Sectional Area, Chimney	None	0.69 cm ² (0.11 in ²)	None	Not Certain that Crevice Cross-Sectional Area is Same As Chimney Cross-Sectional Area
Concentration (Bulk) of Depositing Material	Chloride (from Copper Chloride)	1-10 ppm	None	None

2.2.5.8 Time Dependent, Mass Transfer (Diffusion and Convection) and Chemistry (Hideout and Hideout Return)

Deposition Mechanism: Soluble Material

Source: Cleary, *et al.*,⁽⁵⁾ Part 5 of 5

Output Parameter(s): Mass of Salt Deposited (134-167 mg)

Results

Input Parameters:

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Time	HO HOR	12-16 Weeks 66-96 Days	None	None
Mass or Volume (Bulk)	None	Approx. 1.2 L (0.32 gal)	None	None
Density (Water)	None	Approx. 1.3 g/cc (81.2 lbm/ft ³)	Temperature and Pressure	Obtain from Literature for Concentrated Chemical (Cited Value Here was Back Calculated from Results in Report)
Concentration (Bulk) of Depositing Material	Chloride (from Copper Chloride)	1-10 ppm	None	None
Mass Transfer (Diffusion)	Chloride (from Copper Chloride)	4.6×10^{-7} kg/hr (1.0×10^{-6} lbm/hr)	None	None
Mass Transfer (Convection)	Chloride (from Copper Chloride)	Calculated Above	None	None
Hideout (HO)	Input Output HO	1200 mg (2.64×10^{-3} lbm) 730-750 mg (1.60- 1.65×10^{-3} lbm) 450-470 mg (0.92- 1.03×10^{-3} lbm)	None	None

2.2.5.9 Steady State, Heat and Mass Transfer (Diffusion)

Deposition Mechanism: Soluble Material

Source: Ulke and Goldberg⁽²¹⁾

Description: This model provides a connection between velocities of liquid and gaseous phases, heat transfer, concentration of chemical species in liquid phase, porosity and particle diameter of deposit. This model considers a slab of porous medium on a horizontal non-porous surface, both underwater. Heat is provided by a vertical tube inserted into the porous medium. Vapor flows vertically upward in the porous medium, and the liquid is replenished by counterflow. Five first order differential equations are used including the continuity equations for the liquid and vapor phases, the transformed momentum equation (Kozeny-Karman equation for permeabilities) for the liquid and vapor phases and the change in concentration of chemical species in the liquid along the depth of the porous medium.

Assumptions: Relative laminar and turbulent permeabilities are obtained from other sources (equations included in this reference). Deposit is fully developed and frozen in time.

Successful Applications: Results compared to data obtained by Eckert.⁽²⁰⁾

Limitations: The Thom's formula (convective two phase heat transfer) is used to describe the boiling heat transfer instead of heat pipe heat transfer mechanisms. Thom's equation describes nucleate boiling on a clean surface. This was applied inside a steam chimney, requiring a correction factor for porosity. In the heat pipe theory, the pumping power between the condenser zone (the outside surrounding fluid) and the evaporator (the inside of the chimney) are provided by the capillary force of the deposit capillaries (pressure drop calculated with a modified Darcy's law).

Significant Application Observations: None

Possible Refinements: None

Assessment for Fossil Plant Application: This is a relatively simple model that is attractive. The temperatures are lower than the fossil plant application. Values are given for very few of the input parameters.

Output Parameter(s): Concentration in Porous Media, Capillary Pressure, Capillary Field Flow, Capillary Temperature

Results

Input Parameters:

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Heat Flux	None	10–60 kW/m ² (22- 132 BTU/hr- in ²)	None	Eckert Data
Mass/Volume (Bulk)	None	Not Cited in Reference	None	None
Temperature	None	Probably 300°C (572°F)	None	Nuclear Plant Application for Steam Generator Sludge
Subcooled Boiling	None	Not Cited in Reference	None	None
Pressure	None	Not Cited in Reference	None	None
Velocity	None	Not Cited in Reference	None	None
Density (Steam)	None	Not Cited in Reference	None	None
Density (Water)	None	Not Cited in Reference	None	None
Heat of Vaporization	None	Not Cited in Reference	None	None
Particle Size	None	Not Cited in Reference	None	None
Deposit Porosity	None	Not Cited in Reference	None	None
Concentration of Contaminants in Bulk Liquid	None	Not Cited in Reference	None	None
Convective Mass Transfer	None	Not Cited in Reference	None	None

2.2.5.10 Time Dependent, Heat Transfer and Chemistry

Deposition Mechanism: Soluble Material

Source: Gonzales and Spekkens⁽²²⁾

Description: This model was designed to evaluate the change of concentration of solute in bulk (exponentially decreasing with time) as a result of deposition at the bottom of nuclear steam generators (sludge pile). Tests were performed with sodium chloride. A concentration coefficient is introduced as a multiplier to heat flux and heat transfer area to adjust the calculation to the experimental results. That concentration coefficient could be interpreted as the fraction of heat flux transferred under the sludge pile and transformed in steam, or the fraction of the heat transfer area that is actively generating steam. Connection is made between bulk fluid concentration, heat flux, heat exchange surface and the concentration of fluid in a sludge pile.

Assumptions: All heat transfer under the sludge pile is spent in steaming.

Successful Applications: Although the results were obtained on an experimental test loop and applied to nuclear steam generators in Canada (Bruce 1), the success of the application is not presented in the reference. The sludge and deposits were obtained from the sludge pile u-bend area of the Bruce 1 steam generator. The sludge was packed into a holder by tapping and vibration to obtain different porosities. The 12-cm (0.39-ft) deep sludge pile at Bruce 1 was reported to be “rock hard” despite AVT chemistry control.

Limitations: While experimental results present the influence of depth of deposit and porosity on concentration factor of soluble species in deposit, no attempt is made to connect analytically those parameters.

Significant Application Observations: The rate of concentration change is an exponential function of the heat transfer area and the heat flux. In these experiment when heat transfer was terminated, the diffusion rate of soluble material from the deposit into the bulk fluid was slower than that from the bulk fluid into the deposit when the power was being applied. The change of phase of the solute inside the deposit is an important phenomena, changing the properties and the behavior of the deposit.

Possible Refinements: None

Assessment for Fossil Plant Application: The model appears to be useful for fossil plant application. Extrapolation from the lower temperatures would be required.

Output Parameter(s): Concentration in Porous Media (Concentration Factor = 10^3 – 10^5 Sodium and Chloride)

Results

Input Parameters:

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Time	None	Up to 100 hours	None	None
Temperature (Bulk)	None	256°C (493°F)	None	None
Surface Temperature	None	310-350°C (590-662°F)	None	None
Heat Flux	None	20-110 kW/m ² (44-242 BTU/hr-in ²)	None	None
Concentration of Contaminants in Bulk Fluid	Chloride	30-100 ppm	None	None
pH	Morpholine	8.5	None	This Parameter May Not Be Used in the Equations
Chemical Additive	Hydrazine	1 ppm	None	This Parameter May Not Be Used in the Equations
Mass/Volume (Bulk)	None	2.7 L (0.71 gal)	None	4 L (1.05 gal) Alloy 600 Autoclave
Porosity	None	43-57%	None	This Parameter May Not Be Used in the Equations
Flow Rate	None	Not Cited	None	None
Heat of Vaporization	None	Not Cited	None	None
Deposit Thickness	None	50 – 150 mm (2–6 in)	None	Sludge Pile
Substrate Surface Area	None	None	None	None

2.2.5.11 Time Dependent, Conservation of Mass, Momentum, Energy (Heat) and Chemical Species

Deposition Mechanism: Soluble Material

Source: Millett and Fenton^(23,24)

Description: This one-directional model contains partial differential equations for conservation of mass, momentum, energy and chemical species. The model describes concentrating in occluded regions of the secondary side of a nuclear steam generator in which heat is transferred from the reactor coolant within the tube to produce steam from water on the outside of the tube. Connections are made between bulk fluid concentration, heat flux, heat exchanger surface, concentration of fluid and the extent of the steam blanketing in a sludge pile under transient and steady state conditions.

Assumptions: The heat flux is treated as a constant volume heat source term (varies in tube axial direction). The overall heat transfer includes a nucleate boiling coefficient within an open ended crevice (tube-to-tube support crevice in a nuclear steam generator). The capillary solution temperature is approximated by the temperature of the steam chimney. Saturation temperature in the steam chimney is a function of the solution composition on the surface of steam chimney. The two-phase flow in capillaries is described by Darcy's Law. The dimensionless time constants for conservation of energy and mass are much smaller than those for the conservation of species. The steady state model can be solved using the equations with time derivatives equal to zero. The transient behavior can be modeled by solving the equations with a quasi-steady state approximation.

Successful Applications: Limited steady state and transient experimental data from Mann and Castle⁽¹⁵⁾ for total sodium chloride in a crevice at various superheat and bulk water concentrations were used to verify the model results. The Mann^(4,15) experiments were performed on carbon fiber packed crevices. Point comparisons with experimental values of Baum⁽²⁵⁾ of wetted length of crevices were performed (with acceptable general agreement).

Limitations: There is limited data for validating such a model.

Significant Application Observations: Tortuosity is a second power contributor to the effective diffusion coefficient in the single-phase capillary solution. Thus, the effective diffusion coefficient is largely different at the beginning and end of a capillary. An average tortuosity can be used in the absence of explicit knowledge of the exact value.

Possible Refinements: None

Assessment for Fossil Plant Application: While this is a first-principle, semi-empirical model, it can be applied to deposition in boiling regions of fossil boilers (coefficients are semi-empirical).

Results

Output Parameter(s): Mass Transfer (Diffusion), Hideout, Concentration in Porous Media (Inlet Concentration Times Concentration Factor 10^5 - 10^8), Capillary Pressure, Capillary Flow Field, Capillary Temperature, Wetted Length (0.05–1 cm or 0.02-0.4 in)

Input Parameters:

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Time	None	1–32 Hours	None	Based on Data of Mann
Heat Flux	None	Not Cited	None	None
Temperature (Bulk)	None	280°C (536°F)	None	None
Surface Temperature	None	308°C (586°F)	None	None
Subcooled Boiling	None	5-65°C (9-117°F) Superheat	None	None
Pressure	None	551 N/cm ² (771 psi)	None	None
Viscosity (Liquid)	None	Not Cited	None	None
Viscosity (Steam)	None	Not Cited	None	None
Density (Steam)	None	0.032 g/cm ³ (2.0 lbm/ft ³)	None	None
Density (Water)	None	Not Cited	None	Use Handbook Value for Saturation Temperature in Deposit
Heat of Vaporization	None	1557 J/g (6.69x10 ² BTU/lbm)	None	None
Deposit Surface Area	None	0.125 cm ² (0.0193 in ²)	None	Area of Crevice
Deposit Porosity	None	60%	None	None
Capillary Crossectional Area	None	Not Cited	None	None
Capillary Length	None	Not Cited	None	None
Single Phase Permeability	None	0.1 Darcy	None	At Operating Temperature

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Tortuosity	None	Not Cited	None	None
Thickness	None	1 cm (0.4 in)	None	Crevice Thickness
Diffusion Coefficient	None	$8 \times 10^{-5} \text{ cm}^2/\text{s}$ ($1.2 \times 10^{-5} \text{ in}^2/\text{s}$)	None	None
Concentration of Contaminants in Bulk Liquid	Chloride	10-1,000 ppm/hr	None	None
Diffusion Mass Transfer	None	Not Cited	None	None

2.2.5.12 Steady State, Mass and Heat Transfer with Concentration of Chemicals in Deposit

Deposition Mechanism: Soluble Material

Source: Baum, *et al.* ⁽²⁵⁾

Description: This model describes one-dimensional counterflow of liquid and vapor in a porous medium with upward flow of vapors balancing the downward flow of liquid. The model contains one-dimensional partial differential equations describing conservation of mass, momentum (Darcy's Law) and energy. The model describes the connection between bulk fluid concentration, including inhibitors, heat flux, heat exchange surface, crevice hideout and the extent of the steam blanket in a sludge pile.

Assumptions: The model assumes steady state conditions.

Successful Applications: Large volume of data collected from laboratory experiments for deposition (HO) in crevices followed by HOR of sodium and calcium species at shutdown and during soaking and flushing with deionized water. Low- and high-temperature soaks were included.

Limitations: Computer model predicted wetted length 10x smaller than measured in one experiment.

Significant Application Observations: Both analysis and model indicate little HOR until power reduced below 50%.

Possible Refinements: None

Assessment for Fossil Plant Application: This one-dimensional model has merit for HOR because the tested crevice was made for in-situ oxide growth (in addition to packing of the crevice). The heat tube was Alloy 600, but the oxide grew from carbon steel.

Results

Output Parameter(s): Wetted Length (0.01-0.36 cm or 0.004-0.14 in), Hideout Return (0.028-0.160 M Na and 0.046-0.348 M Cl), Elevation of Temperature in Deposit (Boiling Point Elevation, 0-50°C or 0-90°F), Deposit Permeability, Capillary Pressure, Capillary Field Flow

Input Parameters:

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Time	None	3000 Hours	None	This Value is Not Use in Equations for Steady State
Heat Flux	None	126 kW/m ² (40,000 BTU/hr-ft ²)	None	None
Temperature (Bulk)	None	326°C (620°F)	None	None
Pressure	None	141 kg/cm ² (2200 psi)	None	None
Flow Rate	None	0.2-6 cm ³ /min (7x10 ⁻⁶ – 2x10 ⁻⁴ ft ³ /min)	None	This Parameter May not Be Used in Equations
Viscosity (Liquid)	None	Not Cited	None	None
Viscosity (Steam)	None	Not Cited	None	None
Density (Steam)	None	Not Cited	None	None
Density (Water)	None	Not Cited	None	None
Heat of Vaporization	None	Not Cited	None	None
Deposit Surface Area	None	Gap = 0.0002-0.0005 inch (0.005 – 0.013 mm)	None	None
Deposit Porosity	None	16.8-32.8%	None	None
Capillary Crossectional Area	None	Pore Size = 0.075-3 micron (2.9-115x10 ⁻⁹ in)	None	None
Capillary Length	None	Not Cited	None	None

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Concentration of Depositing Material	Boric Acid and Calcium Hydroxide	Concentration Factor 10^5 - 10^8	None	This Parameter May Not be Used in Equations
Deposit Composition	None	50% Natural Magnetite and 50% Synthetic Magnetite	None	This Parameter May Not be Used in Equations
Thickness	None	0.75 inch (1.9 cm)	None	None

2.2.5.13 Time Dependent, Mass and Heat Transfer with Neutron Flux and Chemistry

Deposition Mechanism: Insoluble Material

Source: Charlesworth⁽²⁶⁾

Description: This work investigated deposition of insoluble substances on a heated surface considering the rate of deposition and the rate of iron release. The deposition rate is proportional to the concentration of insoluble material in the bulk fluid according to this model, and the release rate is proportional to deposit weight. The connection between iron concentration in the bulk coolant, heat flux, heat exchange surface, surface concentration of deposited iron, and deposition rate and release rate on heated surfaces is presented. Tests were conducted in a nuclear test reactor in Canada (Chalk River). Both “in reactor” and “out of reactor” tests were performed under heat flux conditions. The “in reactor” results also have contribution from neutron and gamma ray flux, in addition to heat flux. The deposits were relatively uniform and proportional to square of heat flux in the “out of the reactor” tests. Within the reactor, deposition was proportional to heat flux to a power of 1-5.5, indicating the possibility of significant contribution from gamma and/or neutron flux.

Assumptions: Heat flux and iron concentration in the bulk fluid are the primary factors which determine iron oxide deposit per unit area of heated surface. There is a time until the deposit per unit area reaches a constant value, at which time the deposition and release rates are equal. The deposition process was assumed to be reversible to a point, and the amount of deposit was assumed to decrease if conditions became less favorable for deposition. Densification may eventually result in a dense deposit that cannot be removed.

Successful Applications: This is a semi-empirical model that describes the results of testing in a test reactor.

Limitations: Deposition is described for iron on nuclear fuel elements. Although it may be possible to differentiate between deposition contribution from heat flux and neutron/gamma-ray flux, the combination of general and local thermal-hydraulic and neutronic/gamma conditions add some uncertainty to the selection of the proper exponent to apply to the

Results

contribution of heat flux. Also, the author notes that there may be some unintended impact of irradiation on deposit properties (for example, a change in oxidation potential). Finally, there was limited information on transient deposition and release of insoluble materials on heated surfaces. Heat flux is a term in the deposition process, but is not considered in the release process.

Significant Application Observations: The author concluded that neutron and gamma flux was relatively insignificant to the deposition process in these tests. However, several other parameters were changed, and in some cases the test geometry (serial test section arrangement) may have had an unintended impact on the results.

Possible Refinements: None

Assessment for Fossil Plant Application: The model is simple and of high practical value in combination with other models. The experimental data is provided, and a reassessment of the test results should be performed before using this model.

Output Parameter(s): Removal Rate for Solids and Deposition Rate for Solids ($0.16 \text{ kg/cm}^2\text{-hr}$ or $2.3 \times 10^{-2} \text{ lbm/in}^2\text{-hr}$) [Deposition In Reactor $<10\text{--}4800 \text{ micrograms/cm}^2$ $1.4 \times 10^{-4}\text{--}6.8 \times 10^{-2} \text{ lbm/in}^2$ and Deposition Out of Reactor $10\text{--}5600 \text{ micrograms/cm}^2$ $1.4 \times 10^{-4}\text{--}7.9 \times 10^{-2} \text{ lbm/in}^2$]

Input Parameters:

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Time	None	620-3000 Hours	None	None
Heat Flux	In Reactor Out of Reactor	950-1,400 kW/m^2 (2,090- 3,080 BTU/hr-in^2) 350-1,250 kW/m^2 (770- 2,750 BTU/hr-in^2)	None	None
Velocity	In Reactor Out of Reactor	215-490 $\text{g/cm}^2\text{-s}$ (3.20-6.95 $\text{lbm/in}^2\text{-s}$) 75-410 $\text{g/cm}^2\text{-s}$ (1.06-5.87 $\text{lbm/in}^2\text{-s}$)	None	This Parameter May Not Be Used in Equations

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Chemical Addition	Ammonia	0-24 ppm	None	None
	Hydrogen (In Reactor)	0.03-4.5 ppm		
	Oxygen (In Reactor)	0.01-0.12 ppm		
	Oxygen (Out of Reactor)	0.5-1.7 ppm		
	Iron (In Reactor)	0.01-12 ppm		
	Iron (Out of Reactor)	0.01-2.5 ppm		
Concentration of Depositing Material in Bulk Liquid	None	<10-120 ppb	None	None

2.2.5.14 Time Dependent, Heat Flux with Chemistry and Corrosion

Deposition Mechanism: Insoluble Material

Source: Tomlinson, *et al.* ⁽²⁷⁾

Description: This model describes (a) deposition of magnetite as a function of heat flux, (b) rate of corrosion as a function of temperature, (c) mechanisms for double and triple oxide layer formation and (d) deposition as a function of the difference in the concentration of soluble iron in the bulk liquid and the solubility of magnetite. An empirical connection is made between metal oxide deposition rate and soluble ion supersaturation at the deposit surface. Also, an empirical connection is made between deposit thickness and heat flux and between thickness of metal loss (thickness of oxide formed) and time at various heat fluxes up to 660 kW/m² (1,452 BTU/hr-in²). The deposit thickness is expressed both as a result of soluble metal deposition from bulk solution due to heat flux, and increased oxide thickness through oxidation of base metal.

Assumptions: Magnetite deposition on test samples under heat flux can be obtained through averaging values of a large number of measurements to address for differences in local conditions along the test section. The deposition and corrosion mechanism is postulated to produce three layers. The outer layer results from deposition of magnetite. The inner layer results from corrosion of the base metal. The middle layer is predominantly magnetite and results from outward diffusion of Fe²⁺ and inwardly diffusing O²⁻ or water.

Successful Applications: The model was developed from laboratory testing.

Results

Limitations: Empirical corrosion correlations obtained from data on limited types of cold-rolled tubing (2.25Cr-1Mo and 9Cr-1Mo). No apparent connection is made between the triple-layer corrosion mechanism and the proposed formulas for thickness of magnetite deposited (outer layer) or the metal loss formulas from the base metal to form the inner oxide layer. The author indicates wide scatter in the data (error bars are shown in the reference).

Significant Application Observations: Corrosion rate was independent of heat flux up to approximately 660 kW/m^2 ($1,452 \text{ BTU/hr-in}^2$), but it decreased at higher heat flux (outer layer diffusion is proposed to be rate limiting). An exponent of 4.3 was assigned to the heat flux for determination of the thickness of deposition of magnetite based on a curve fit that gave most weight to data for $660\text{-}860 \text{ kW/m}^2$ ($1,452\text{-}1,892 \text{ BTU/hr-in}^2$) or (this is higher than fossil plant application). Only 2 of 10 data points were collected in the range of $250\text{-}440 \text{ kW/m}^2$ ($550\text{-}968 \text{ BTU/hr-in}^2$).

Possible Refinements: None

Assessment for Fossil Plant Application: The base metal material is applicable to portions of fossil boilers. The equations appear to be applicable, but the temperature is lower than that in fossil plants.

Output Parameter(s): Deposition Rate for Solids and Deposit Thickness

Input Parameters:

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Time	None	1030-4280 Hours	None	None
Temperature	None	350°C (662°F)	None	None
Heat Flux	None	0-860 kW/m^2 (0-1,892 BTU/hr-in^2)	None	None
Velocity	None	357-2,570 $\text{kg/m}^2\text{-s}$ (0.51-3.6 $\text{lbm/in}^2\text{-s}$)	None	This Parameter May Not be Used in Equations
Tube Inside Diameter	None	15.7-20.4 mm (0.62-0.81 in)	None	Flow Was Inside of the Tube This Parameter May Not be Used in Equations
Pressure	None	179 kg/cm^2 (2,550 psi, 17.6 MPa)	None	This Parameter May Not be Used in Equations

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Blowdown	None	1%	None	Through Ion Exchange Columns This Parameter May Not be Used in Equations
Concentration of Contaminants in Bulk Liquid	TDS Silica Copper Chloride Oxygen	<50 ppb <2 ppb <2 ppb <10 ppb <7 ppb	None	Note sodium chloride (1-3 ppm), sodium sulfate (2 ppm) and sodium hydroxide (7 ppm) were present during parts of certain tests. Higher than specified oxygen was present during one test. This Parameter May Not be Used in Equations
Chemical Additives	None	Not Cited	None	AVT Used in All Tests This Parameter May Not be Used in Equations
Concentrating of Depositing Material	Iron	<10 ppb	None	None

2.2.5.15 Steady State, Heat and Mass Transfer with Chemistry

Deposition Mechanism: Soluble Material

Source: Ashmore, *et al.* ⁽²⁸⁾

Description: Although this is primarily a corrosion model, the results are significant because the corrosion tests (and equations that describe the results) were performed under low and high heat flux conditions and in the presence various thicknesses of in-situ produced deposit. Additionally, the impact of small defects on deposition and corrosion are presented. The model describes magnetite solubility as a function of dissolved hydrogen concentration. Empirical relationships show metal thickness corroded as a function of HCl concentration in solution and crystal size as a function of magnetite deposit thickness. Theoretical correlation is presented between magnetite solubility and hydrogen ion content, temperature and ECP of the bulk solution. The tube metal compositions were 2.25Cr-1Mo and 9Cr-1Mo. The corrosion impact was highest on tubes with dissimilar metal welds as a result of the galvanic

Results

couple and difference in thermal conductivity (30% difference in heat flux at a few millimeters upstream of the weld junction).

Assumptions: Very small localized geometrical configurations, such as weld bead, weld rings and tube defects, may impact deposition and corrosion. The impacts may result from very local changes in heat flux, fluid flow and other parameters and, as such, affect the localized connection between the deposition and corrosion.

Successful Applications: The data were generated in laboratory tests carried out on tubing that is similar to that used in fossil boilers. Data on corrosion and deposition due to some small geometrical changes were thoroughly explored. A correlation was observed between magnetite crystal size and magnetite deposit thickness in localized defects.

Limitations: The equations do not have terms for heat flux, deposit thickness and extent of flaws. Magnetite deposition and corrosion is not explicitly connected to the heat flux. The empirical correlation between thickness of metal corroded and HCl concentration in bulk solution does not consider metal surface time of exposure to HCl, explicitly

Significant Application Observations: Accumulation of crystalline magnetite was shown to be higher downstream of a weld. The weld was a step change of 1 mm or 0.04 in (axial direction), and the result was a 3 mm or 0.12 in wide accumulation of magnetite crystals stacked upon each other. The average size of the crystals on the top surface of the deposit was 90 microns (0.0035 in). Metal loss under the deposit was higher near the weld.

Possible Refinements: Combine with heat and mass flux models.

Assessment for Fossil Plant Application: Local flow disturbances have been found to be associated with a significant fraction of boiler tube failures in fossil plants.

Output Parameter(s): Metal Ion Dissolved (50-450 ppb, Nernst) and Metal Loss from Corrosion

Input Parameters:

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Time	None	400-3200 Hours	None	Time not explicitly included, while being implicitly considered as the residence time of the concentrated HCl solution at metal surface. Residence time was not quantified.

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Heat Flux	None	660 kW/m ² (1,452 BTU/hr-in ²)	None	Locally Changed 30% as a Result of Local Changes in Geometry This Parameter is Not Used in Equations
Temperature	None	325-370°C (617-698°F)	None	None
Pressure	None	179 kg/cm ² (2,550 psi, 17.6 MPa)	None	This Parameter is Not Used in Equations
Velocity	None	1 m/s (39 in/s)	None	This Parameter is Not Used in Equations
Flow Rate	None	0.19 kg/s (3.0 gal/min)	None	This Parameter May Not be Used in Equations
Extent of Flaw	Diameter Depth Sharp Step Change in Tube Diameter	Max of 250 micron (0.0098 in) Max of 750 micron (0.0295 in) 170 micron (0.00669 in)	None	This Parameter is Not Used in Equations
pH	None	5.8	None	Hydrochloric Acid
Concentration of Contaminant	Hydrochloric Acid	2-4 ppm	None	None
Concentration of Depositing Material	Iron	132 ppb	None	None
Hydrogen Diffusion	None	140-200 ppm	None	Diffusion Through Tube Wall This Parameter May Not be Used in Equations
Hydrogen	None	181 ppb	None	This Parameter Not Used in Equations
Chemical Additive	Ammonia Hydrazine	0.7 ppm 0.15 g/min (0.00033 lbm/min)	None	This Parameter is Not Used Directly in Equations

Results

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Contaminants	Aluminum Nickel Chromium Magnesium Copper Manganese Silica	1 ppb 2 ppb 1 ppb 4 ppb 2 ppb 25 ppb 11 ppb	None	This Parameter is Not Used in Equations
Weld Hardness	None	270 Vickers	None	This Parameter is Not Used in Equations
Corrosion Current Density	None	Not Cited	None	None
Tube Inside Diameter	None	20.1 mm (0.791 in)	None	This Parameter is Not Used in Equations

2.2.5.16 Steady State and Time Dependent, Mass and Heat Transfer with Chemistry (Concentration and Solubility)

Deposition Mechanism: Insoluble Material

Source: Burrill⁽²⁹⁾

Description: This model describes the deposition and release rates of metal oxide corrosion products onto heated and non-heated surfaces and under boiling and non-boiling conditions. Equations describe tests conducted in a light-water test reactor (X-3, Chalk River) and in a heavy-water test reactor (CANDU Nuclear Power Demonstration, NPD). The model combines equations for deposition and release to predict deposit weight (input parameters for deposition and release are combined in the following table, but are separated in the discussion in Section 3 of this report). Release of insoluble material is assumed to be by chemical dissolution, only. Tests were conducted under boiling and non-boiling conditions in the 25 MWe CANDU, heavy water (D₂O) test reactor with Zircaloy-2 pressure tubes containing nine fuel bundles. The fuel was natural enrichment uranium oxide (UO₂). The purpose of these experiments was to determine if a CANDU reactor could operate under boiling conditions. Deposits were composed of magnetite (Fe₃O₄) near the inlet of the fuel channel and hematite (α -Fe₂O₃) elsewhere. Other metals composed <10% of the deposit and included Ni, Cu, Cr, Co and Mn. Lithium hydroxide (LiOH) or aqueous, deuterated ammonia (ND₃) were used for pH control. The ammonia addition produce high concentrations of deuterium (D₂) and nitrogen; the dissolved deuterium, an isotope of hydrogen (H₂), may have participated in the chemistry of the deposition and release.

Assumptions: Since release of insoluble material is assumed to be by dissolution, the dissolution equation has terms for both soluble and insoluble material. The solubility is taken from an equation that describes the work of Sweeton and Baes.⁽³⁰⁾ The deposition rate equation is written with a term for insoluble (particulate) material.

Successful Applications: Plots of experimental data for deposit weight (g Fe/m^2 lbm/Fe/in^2) appeared to be well behaved functions of surface heat flux in the range of about 200-900 kW/m^2 (440-1,980 BTU/hr-in^2). The deposition appeared to be linear up to about 900 kW/m^2 (1,980 BTU/hr-in^2) in light-water tests and up to about 300 kW/m^2 (660 BTU/hr-in^2) in the heavy-water tests, with some curvature at high heat flux. However, agreement with the model predictions was only within about an order of magnitude. This may reflect a weakness in the mode or in the measurement of deposition. The steady-state predictions for deposit were acceptable for heated surfaces.

Limitations: Heat flux is only considered in the equations that describe release of insoluble material (dissolution). Heat flux is not a term in the deposition equation. There is no velocity term in the mass transfer equations. The mass transfer coefficient for lithium hydroxide appears to have been applied to all species in solution, including the metal oxide particles. Although lithium hydroxide solubility is considered, no term is included for the distribution of ammonia between steam and water under boiling conditions.

Significant Application Observations: Heavy deposits ($>35 \text{ g/m}^2$ or $>5 \times 10^{-5} \text{ lbm/in}^2$) were found under boiling conditions compared to non-boiling tests. The boiling tests were performed with ammonia for pH control, and the non-boiling tests were performed with lithium hydroxide. The hydrogen concentration increased to 40 $\text{cm}^3/\text{kg H}_2\text{O}$ ($6.4 \times 10^{-4} \text{ ft}^3/\text{lbm}$) during the boiling tests.

Possible Refinements: Include heat flux in deposition rate (possibly by combining with equations from other investigators).

Assessment for Fossil Plant Application: The equations for the solubility and dissolution predictions would be useful, but the equations for deposition need to be adjusted for the contribution of heat flux.

Output Parameter(s): Deposition Rate for Solids and Removal Rate for Solids (Total Deposition and Removal = 50-34,000 mg/m^2 or 7.1×10^{-5} – $4.8 \times 10^{-2} \text{ lbm/in}^2$)

Input Parameters:

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Time	None	31-560 Effective Full Power Days (EFPD)	None	None

Results

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Temperature	Inlet (Heavy Water) Outlet (Heavy Water) Inlet (Light Water) Outlet (Light Water)	247-251°C (477-484°F) 271-277°C (520-531°F) 286-288°C (547-550°F) 293°C (559°F)	None	None
Heat Flux	Beginning of Test (Heavy Water) End of Test (Heavy water) Maximum (Light Water)	0-810 kW/m ² (0-1,782 BTU/hr-in ²) 0-500 kW/m ² (0-1,100 BTU/hr-in ²) 400-1,140 kW/m ² (880-2,508 BTU/hr-in ²)	None	Heat Flux Lower After Test
Pressure	Boiling (Heavy Water) Non-Boiling (Heavy Water)	58 kg/cm ² (825 psi, 5.70 MPa) 75 kg/cm ² (1065 psi, 7.34 MPa)	None	This Parameter May Not Be Used in Equations
Flow Rate	Boiling Non-Boiling	307 kg/s (676 lbm/s) 648 kg/s (1,428 lbm/s)	None	This Parameter is Not Used in Equations
Steam Quality	Average (Heavy Water) Maximum (Heavy Water) Light Water	12% 16% 6-7%	None	None
Cross-Section Flow Area	None	3.52 cm ² (0.55 in ²)	None	Not Used Directly in Equation
Equivalent Hydraulic Diameter	None	.37 cm (0.15 in)	None	Not Used Directly in Equation
Reynolds Number	None	10 ⁵	None	Not Used Directly in Equation

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Results

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
pH	None	8.4-10.2	None	This Parameter is Not Used Directly in the Equations
Concentration of Contaminants in Bulk Liquid	Oxygen Lithium	<10 ppb 0.2-2.0 ppm	None	Also, See Above Listing of Chemical Treatment Conditions
Concentration of Depositing Material	Particles (Primarily Iron Oxide) Lithium	1.8 ppb Calculated	None	Equation Given to Calculate Concentration in Deposit Using Concentration in Bulk
Solubility Constant	a ₁ a ₂ a ₃	4.21×10^{-13} -4.00×10^{-10} 1.006×10^{-7}	Temperature, T, in Degrees Celsius $S = a_1 T^2 + a_2 T + a_3$	Curve Fit Constants for Sweeton and Baes ⁽³⁰⁾

2.2.5.17 Time Dependent, Heat Transfer and Chemistry

Deposition Mechanism: Soluble Material**Source:** Mizuno, *et al.*⁽³⁰⁾

Description: Data were collected from operating subcritical and supercritical fossil boilers at power plants in Japan. The plants have condensate demineralizers. Plant metallurgy includes copper-nickel, carbon steel and stainless steel. The ratios of metals in feedwater are presented. This reference contains relevant data with minimal first principle equations. Deposition rate constants and amounts of deposit are plotted as a function of heat flux. Also, the amount of deposition of hematite is plotted as a function of time.

Assumptions: Plant data can be used to correlate deposition as a function of operating parameters.

Successful Applications: Not applicable.

Limitations: The use of plant data is complicated by concurrent changes in contributing factors. Also, operating conditions and plant chemical treatment are not clearly defined in the reference. In some case, the measured deposition rate exceeded the total amount of feedwater iron, indicating that corrosion iron may also be included in the reported values for deposition.

Significant Application Observations: Deposition was found to be linear with heat flux on samples removed from operating plants, although some corrosion iron may have been included in the measurement. The amount of deposition was higher in nucleate boiling than in subcooled boiling regions. The insoluble corrosion products in the feedwater were similar to higher soluble corrosion products during full load, steady state operation. The insoluble fraction increased during transients. Deposition on the inside of tubes was larger on the fire side of the tube. Nickel plating did not show consistent improvement in reducing deposition, and in some cases, had higher deposition.

Possible Refinements: Re-plot data to obtain empirical curve fits for possible use in aggregate model within the aforementioned limitations.

Assessment for Fossil Plant Application: The data were obtained from operating power plants.

Output Parameter(s): Deposition Rate (50-500 kg/yr or 110-1,100 lbm/yr) and Mass Deposited ($10\text{-}30\text{ mg/cm}^2$ or $1.4\text{-}4.3 \times 10^{-4}\text{ lbm/in}^2$)

Input Parameters:

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Time	None	19,000 Hours	None	Tube Sections Removed for Examination
Concentration (Bulk)	Subcritical - Iron, Copper and Nickel Supercritical - Iron	Concentration Not Cited Explicitly (Low and High) – Nickel Ferrite and Magnetite Drum Unit, 156 MW 3 g/hr Fe (0.0066 lbm/hr) 1 g/Cu (0.0022 lbm/hr) 2.4 g/hr Ni (0.0053 lbm/hr) Soluble-to- Insoluble = 1-10	None	Produced in Plant from Pre-Boiler Components (Condenser, Feedwater Heaters, Deaerator, etc.) 50-500 kg/yr (110-1,100 lbm/yr)
Heat Flux	None	1-6 kcal/m ² -hr (0.4-2.2 BTU/ft ² - hr)	None	Plotted as Deposition Rate as Function of Heat Flux

Results

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Deposition Rate Constant	None	$1-5 \times 10^{-3}$	None	None
Total Mass of Particles	None	Up to 500 kg/yr (1,100 lbm/yr)	None	

2.2.5.18 Steady State, Chemistry (Steam and Water)

Deposition Mechanism: Soluble Material

Source: Palmer, *et al.*⁽³²⁻³⁷⁾

Description: Experiments were conducted to determine the solubility and speciation of chemicals in high-temperature steam (vaporous carryover) and water. The results are plotted in several papers as a function of reciprocal temperature ($1/T$), density or pH. A general equation is proposed for vaporous carryover, incorporating temperature and steam density as input parameters with constants that depend on the chemical composition. A computerized model was developed to incorporate the portioning constant (distribution ratio), hydrolysis constant and ion product of water to predict the composition of steam and condensate (“early condensate”). The copper oxide tests with CuO and Cu₂O were conducted in the presence of various chemical agents including NaOH, NH₃, B(OH)₃, H₃PO₄, (OHCH₂)₃CNH₂, (OHCH₂)₃CN(OCH₂CH₃)₂, HF₃CSO₃ and HNO₃.

Assumptions: The experimental systems were assumed to be at equilibrium (tests were conducted to confirm that the experiments were at equilibrium). Moisture carryover was treated as an input value to the calculation (moisture carryover is a characteristic of boiler design).

Successful Applications: Results are based on bench-scale experiments (high-temperature flow cells, autoclaves and potentiometric titrations). The model for partition coefficients uses constants derived from experiments and activity coefficients from other sources to calculate the steam and condensate concentrations for those chemicals (including pH and conductivity). Input parameters are concentrations for boiler chemical additives and contaminants. Projections of steam and condensate concentrations are made for target and action level concentrations in the boiler water. The details of the computer model for steam solubility (partition coefficients) were not published in these references and, thus, cannot be fully assessed at this time.

Limitations: The steam solubility tests were conducted in a static mode in a very small test vessel (600-700 mL or 0.16-0.18 gal), limiting the amount of steam that could be removed for sampling. The concentrations of low-volatility solutes had to be significantly higher than those found in steam cycles of power plants in order to obtain sufficient amounts for an accurate analysis. For this reason, independently measured activity coefficients are needed to calculate the portioning constants. Also, the possible impact of system dynamics (kinetics)

on dissolution into and deposition from steam is not included. The calculation method cannot be assessed without additional information.

Significant Application Observations: Plant data for vaporous carryover is generally higher than experimental data, possibly as a result of significant contribution of mechanical carryover according to the authors.

Possible Refinements: Independent benchmarking for vaporous carryover would be useful.

Assessment for Fossil Plant Application: These results are directly applicable to fossil power plants.

Output Parameter(s): Concentration of Chemical In Steam and Water (10^{-2} - 10^5 ppb Cu in Water, 10^{-1} - 10^3 ppb Cu in Steam) – with the Exception of Copper, the Results are Generally Given in Terms of Partition Coefficient without Reporting of Actual Experimental Results for Steam Concentrations

Input Parameters:

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Temperature	Steam – Sodium/ Chloride/Sulfate	25-350°C (77- 662°F)	None	
	Steam – Copper Oxides (CuO and Cu ₂ O)	Up to 440°C (824°F)		
	Water – Copper Oxides (CuO and Cu ₂ O)	25-350°C (77-662°F)		
	Steam – H ₂ PO ₄ ⁻ , HPO ₄ ²⁻ , and PO ₄ ³⁻	250-350°C (482-662°F)		
	Steam – NH ₄ Cl, HCl and NH ₃	100-350°C (212-662°F)		
	Water – Magnetite	100-290°C (212-554°F)		
	Water – Zinc Oxide	50-290°C (122-554°F)		
	Water – Magnesium Hydroxide	60-200°C (60- 392°F)		
	Water – Aluminum Hydroxide	100-290°C (212-554°F)		
	Water – Titanium Oxide	Up to 290°C (554°F)		

Results

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Pressure	Steam - Sodium/ Chloride/Sulfate Steam – Copper Oxides (CuO and Cu ₂ O)	168 kg/cm ² (165 bar, 2,400 psi) 183 kg/cm ² or 2,600 psi (18 MPa at <357°C or 675°F) and Supercritical at >357°C or 675°F)	None	Steam Copper Oxide Data Includes Subcritical Plant Data and Supercritical Bench Tests
Steam Density	Steam – Copper Oxides (CuO and Cu ₂ O)	10 ^{-2.1} –10 ^{-0.2} g/cm ³ (0.5-39 lbm/ft ³)	Temperature and Pressure	
pH	None	2-13	Temperature	pH Has a Significant Impact on the Results pH was Varied over Different Ranges for Different Tests
Concentration of Liquid Concentrate	Steam - HCl, NaCl, NaOH, H ₂ SO ₄ , NaHSO ₄ and NH ₃ Steam - NH ₄ Cl, HCl and NH ₃	Not Cited 2.8-89,000 ppm Cl	Temperature, Pressure and Chemical Composition	
Distribution Ratio (Partitioning Coefficient)	Steam - HCl, NaCl, NaOH, H ₂ SO ₄ , NaHSO ₄ , and NH ₃ Steam - H ₂ PO ₄ ⁻ , HPO ₄ ²⁻ , and PO ₄ ³⁻ Steam - NH ₄ Cl, HCl and NH ₃	10 ⁻¹⁶ –10 ⁴ 10 ⁻⁴ –10 ⁴	Temperature, Pressure and Chemical Composition	Curve Fit Constants for Partitioning Coefficient as a Function of Temperature and Density are Presented for Formic, Acetic and Phosphoric Acids
Equilibrium Constant for Chemical Reactions (Dissociation Constant)	Composition Dependent	Not Cited	None	Data Appear to be Needed for the Computer Calculation

2.2.5.19 Constant Rate, Mass and Heat Transfer with Chemistry (Solubility and Deposition)

Source: Bellows⁽³⁸⁾

Description: This model was designed to predict the deposition rates of water soluble materials (such as sodium chloride and silica) at various locations throughout dry regions of the turbine. This mass transfer model considers homogeneous nucleation, heterogeneous nucleation and solubility. The model contains no adjustable parameters.

Assumptions: Although this model was designed for predicting the deposition of water soluble materials that are dissolved in steam, the model may be more generally applicable to solids dissolved in water.

Successful Applications: The Bellows model agrees with the Lindsay and Lee estimate for sodium chloride deposition in turbines.

Limitations: Uncertainties in steam solubility (30-50%) and molecular diameter (20-30%). Deposition rates may be low as a result of general area modeling.

Significant Application Observations: Deposition at low load may be significant, and deposition may be faster than cleanup.

Possible Refinements: Consider addition of component geometry.

Assessment and Risks for Fossil Plant Application: Applicable to turbines; some uncertainty would be associated with extrapolation of steam/water equations to solid/water equations for boiler application.

Output Parameter(s): Deposition Rate (μ/yr or mils/yr for solids or $\text{mL}/\text{cm}^2\text{-yr}$ $\text{gal}/\text{ft}^2\text{-yr}$ for liquids)

Input Parameters:

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Time	None	Cited for Annual Deposition	None	Constant Rate
Temperature	None	Maximum of 537°C (1,000°F)	None	Cited Temperature is at Turbine Inlet
Pressure	None	163 kg/cm ² (160 bar, about 2,300 psi)	None	Cited Pressure is at Turbine Inlet

Results

INPUT PARAMETER	SUBCATEGORIES	RANGE	DEPENDENT PARAMETER(S)	COMMENTS
Steam Solubility	Sodium Chloride Silica	1–20 ppb <3,000 ppb	Temperature Pressure Steam Density (Function of Temperature and Pressure)	Application to Chemicals Other Than Sodium Chloride and Silica is Possible
Molecular Volume	Water Trace Impurities	Not Cited	Viscosity of Water (Function of Temperature and Pressure) Crystallographic Characteristics for Trace Impurities, Specifically Crystal Density from Waters of Hydration and Geometric Diameter	None
Reynolds number	None	Below 1.3×10^7	Mass Flow Rate, Temperature, Pressure, Velocity	None
Convective Mass Transfer Coefficient	None	None	Hydraulic Diameter and Viscosity	None

2.3 Additional Evaluation of Other Existing Equations

Since the scope of this effort was to establish the feasibility of producing an aggregate model of deposition, it was not necessary to evaluate all of the available equations and models that may be incorporated into the final product. However, a large number of theoretical and semi-empirical equations had previously been assembled by Warwood, Roe and Sears of Montana State University.⁽³⁹⁾ This assembly of theoretical and semi-empirical equations was not assessed in detail under the current feasibility study. However, for completeness a review of these equations was performed to determine the degree of difficulty that may be encountered in development of the aggregate model.

The assessment of these equations consisted of selecting pertinent groups of equations from a much larger set of equations presented in the unpublished work of Warwood, Roe and Sears.⁽³⁹⁾ The selected equations are described in Appendix B, including a listing of the input and output parameters and a general description of the equations. Since the details of the original work were not reviewed, less weight was given to the exact formulation of equations for this assessment. Of special attention in the description of the equations was the degree by which power plant operational parameters influence the outcome of the process described by the equation.

These theoretical and semi-empirical equations may, in some cases, overlap those contained in the experimental equations or models used by investigations that were assessed in more detail in Section 2.2. The equations were segregated into the following subcategories:

- Change of state – thermodynamic changes in deposited materials and changes of crystals in deposits (Appendix B.1),
- Dilute solutions • solvent solute equations (Appendix B.2),
- Transport and diffusion in steam and within deposits (Appendix B.3),
- Adsorption and desorption (Appendix B.4),
- Thermodynamic equations for surfaces - chemistry exchange across phases and concentration in droplets (Appendix B.5),
- Kinetics of deposition (Appendix B.6),
- Potential of Zero Charge (PZC) (Appendix B.7),
- Multilayer deposition (Appendix B.8),
- Particle electric field interaction - particle settling (Appendix B.9),
- Solutions of gases in liquids (Appendix B.10) and
- Non- ideal behavior of a component in solutions (Appendix B.11).

The following observations were made after studying the large number of equations describing individual phenomena related to deposition and change of state in deposits:

1. A theoretical formulation is available for many of the individual phenomena participating in deposition.
2. Physical constants (theoretical and empirical) abound in the equations.
3. Theoretical phenomena described through the aforementioned equations may differ from physical reality, as a result of specific conditions available to define boundary conditions and/or the capability to identify data values for the physical constants in equations from the literature or/and available experiments.
4. Equations describe different facets of the same deposition phenomena (such as change of state, transport, adsorption, desorption and particle field interaction).
5. While separate identification of processes helps the better understanding of individual processes, only the coupling of individual equations will result in a better, more reliable model of natural phenomena.
6. Coupling of equations is performed through boundary conditions.

Even after the preliminary selection of equations that describe only the most pertinent portions of the deposition process, a large number of equations remained in the list presented in Appendix B. The multitude of phenomena impacting deposition and the number of equations required to describe these phenomena require that the aggregate model be developed in stages. Many of the equations in Appendix B may not be used in the initial aggregate model. By contrast, most of

Results

the investigators have found that deposition processes for a specific application can be described through a significantly reduced number of equations (Section 2.2).

3

DISCUSSION

3.1 Assessment of Input Parameters for Aggregate Model

All input and output parameters from the detailed assessment (Section 2.2) were tabulated and ranked according to the information that is known about each parameter. This assessment does not include the additional equations identified in Section 2.3. Note that certain output parameters from one set of equations or model are used as input parameters for another set of equations or model.

Although there are a total of 73 input parameters (including coefficients) and 26 intermediate and final output parameters, the actual number required to exercise a specific calculation to produce the final result ranges from 1 – 22 (Figure 3-1). A limited number of final output parameters are identified for the soluble and insoluble material, including deposition rate, deposit thickness, mass of material deposited, hideout and concentration in porous media.

The initial ranking of 1 – 4 for each input parameter was based on an engineering judgment of the current state-of-knowledge of that parameter, as follows:

- 4 – Parameter that is relatively well known
- 3 – Parameter that is possible to establish or define, but may not be well known
- 2 – Parameter that is more difficult to establish or define
- 1 – Parameter that may be very difficult to establish or define with known certainty

In order to assess the ability to obtain a given output parameter, simple normalization was performed by summing the ranking values for each input parameter that is required for a specific output parameter, in accordance with a specific set of equations or model, and dividing by the total number of input parameters. The output of some equations or models was required as input to other equations or models. Therefore, normalized results for some output parameters were fed into the input calculation for the normalization of other parameters to account for the interrelationship between input and output of various equations and models. The intermediate output parameters are those that are required primarily as input parameters for another calculation (for example, mass transfer coefficient). Output parameters (including intermediate output parameters) frequently have non-integer values, since they result from a calculation. Input parameters have integer values unless they were intermediate output parameters.

Discussion

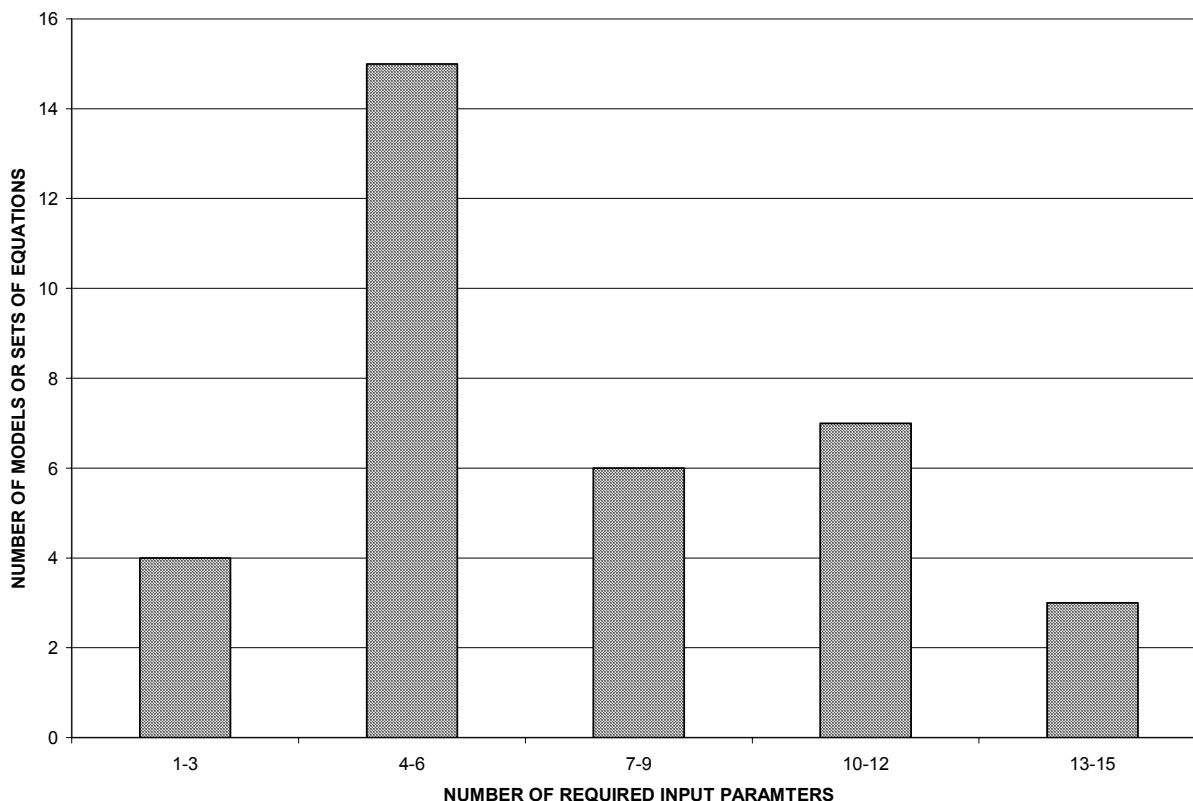


Figure 3-1
Number of Input Parameters Required for Various Models or Equations

The results were then plotted as influence diagrams for soluble and insoluble species (Figures 3-2 through 3-5). Note that soluble and insoluble in this case indicate highly water soluble materials (such as sodium chloride, sodium hydroxide, etc.) and materials that are nearly insoluble in water (metals and metal oxides), respectively. Metal ions and dissolved metals are of the insoluble classification for this discussion because these materials become insoluble in a surface deposit.

This approach has several limitations including the inability of account for the strength of the influence of each input parameter in the equations (for example, second or third order influence or impact of various coefficients on individual terms of the equation). Nevertheless, the approach provides useful insight. The relative impact of each input parameter would be better assessed as part of a sensitivity study once the model is developed.

The rankings of 1 – 4 are converted to percentages in subsequent discussions. These percentages represent the fraction of input parameters and coefficients that are known. These percentages do not represent a probability of success.

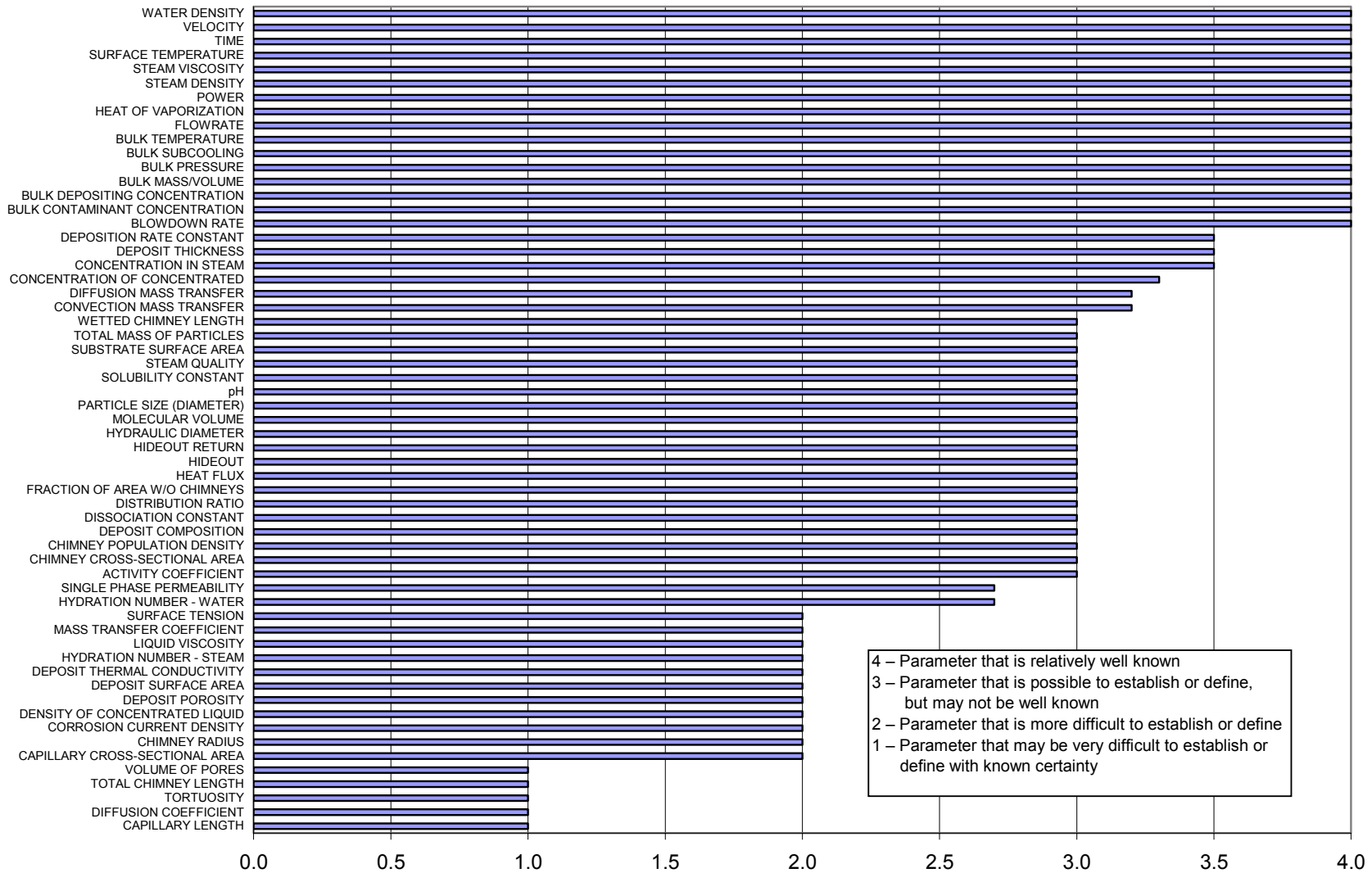


Figure 3-2
Input Parameter Rankings for Soluble Material

Discussion

FINAL RESULTS

MASS OF MATERIAL DEPOSITED
DEPOSITION RATE
CONCENTRATION IN POROUS MEDIUM
HIDEOUT

INTERMEDIATE RESULTS

CONCENTRATION IN STEAM
METAL LOSS FROM CORROSION
METAL ION DISSOLVED
CAPILLARY TEMPERATURE
DIFFUSION MASS TRANSFER
CAPILLARY PRESSURE
CAPILLARY FLOW FIELD
CONVECTION MASS TRANSFER
POST-DEPOSITION SURFACE TEMPERATURE
PRESSURE DROP IN STEAM CHIMNEY
DRY-OUT HEAT FLUX
WETTED LENGTH
BOILING POINT ELEVATION
DEPOSIT PERMEABILITY
MASS TRANSFER COEFFICIENT - DIFFUSION
TIME CONSTANT

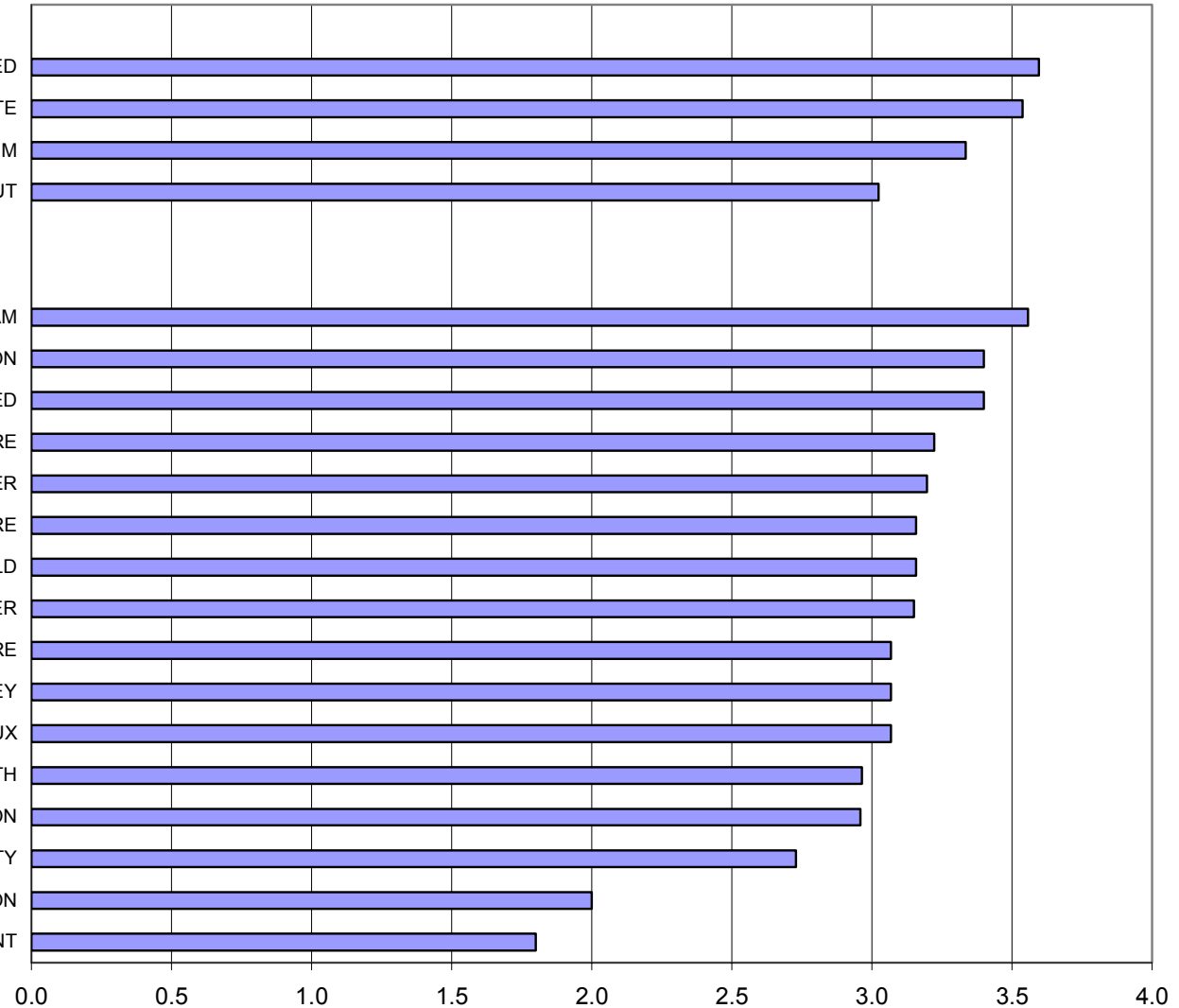


Figure 3-3
Output Parameter Rankings for Soluble Material

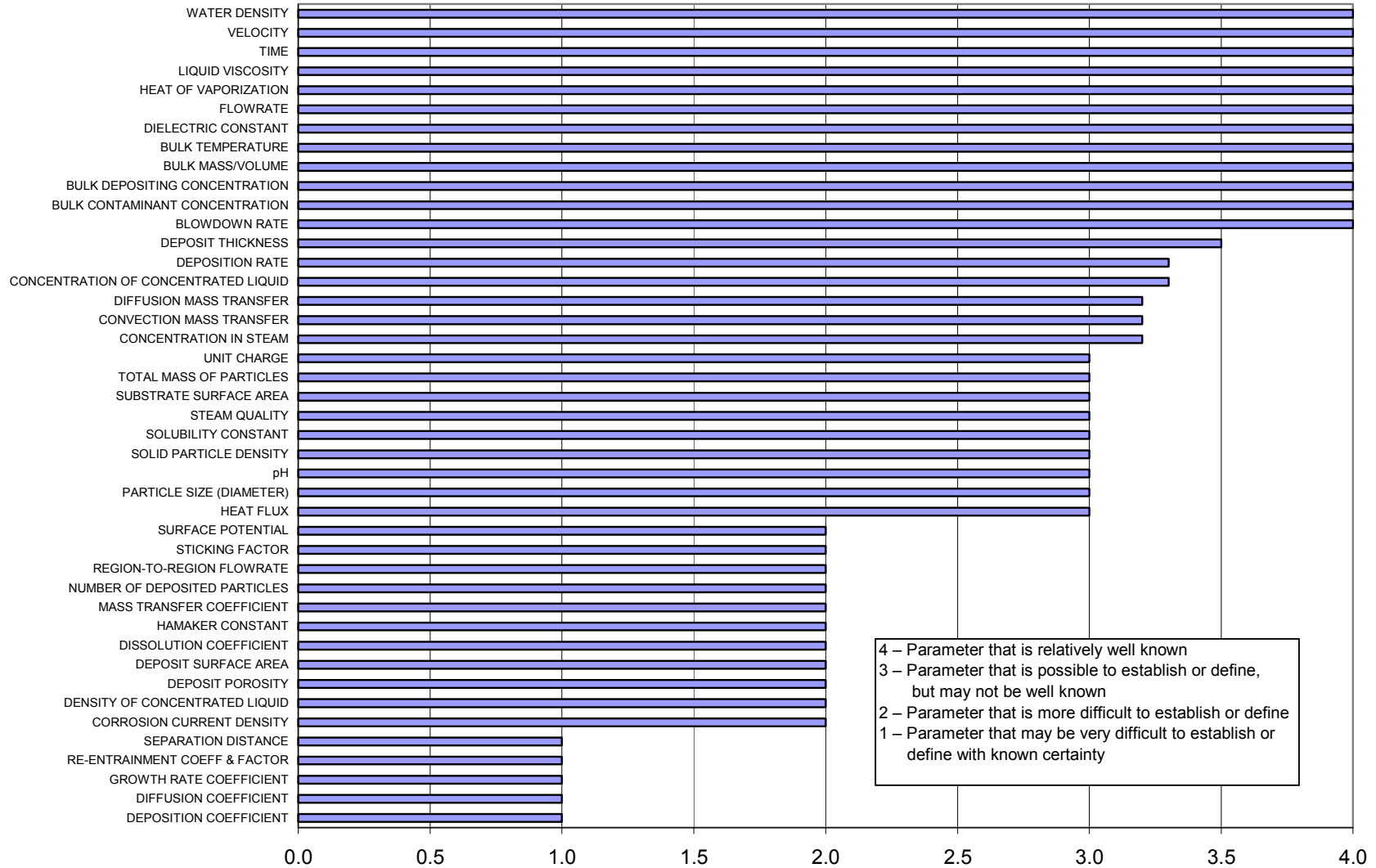


Figure 3-4
Input Parameter Rankings for Insoluble Material

Discussion

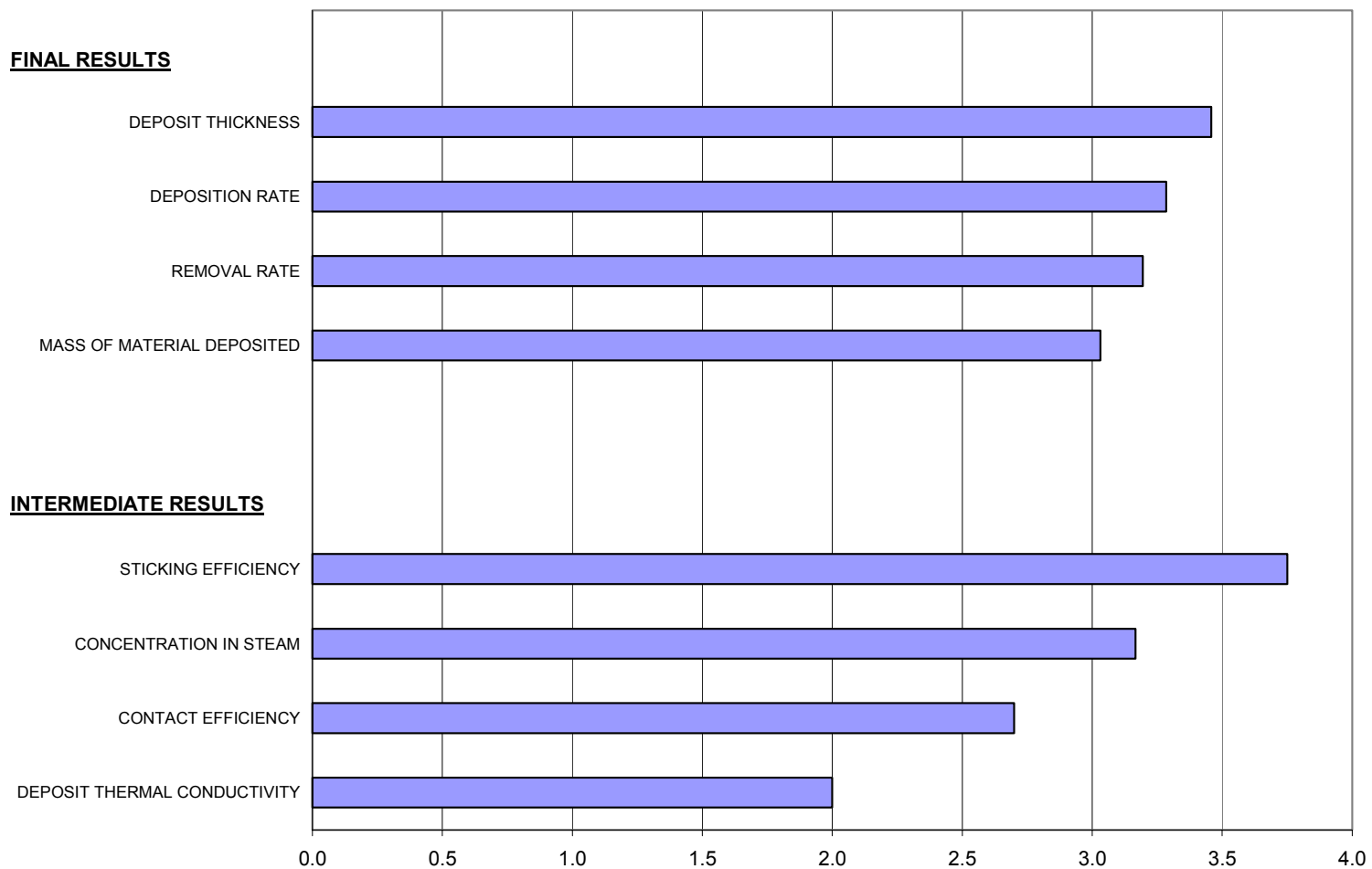


Figure 3-5
Output Parameter Rankings for Insoluble Material

The ranking of the final output parameters on the scale of 1 – 4 is as follows for insoluble material (metals and metal oxides):

- Mass of Material Deposited 3.0 (76%)
- Deposition Rate 3.3 (82%)
- Deposit Thickness 3.5 (86%)
- Removal Rate 3.2 (80%)

The ranking of the final output parameters on the scale of 1 – 4 is as follows for soluble material (sodium chloride, etc.):

- Hideout 3.0 (76%)
- Mass of Material Deposited 3.6 (90%)
- Concentration in Porous Media 3.3 (83%)
- Deposition Rate 3.5 (88%)

Information required for prediction of the impact of deposits on performance was ranked as follows:

- Post-Deposition Surface Temperature 3.2 (80%)
- Post-Deposition Heat Flux 3.2 (80%)

3.2 Overlapping Input/Output Parameters and Missing Information and Data

Overlapping input and output parameters were identified for each model or set of equations to determine the ability to merge the independent modules into a comprehensive model. The output parameters can compliment each other, extending the characterization of the deposition, or refer to the same output parameter, identifying a conflict in the output. Overlap was found for many of the intermediate and final output parameters. The final aggregate model can address these items by selecting the most appropriate data for the application or by allowing user selected options.

The following overlapping final output parameters were found for insoluble material:

- Mass of Material Deposited – None
- Deposition Rate – 4 Models or Sets of Equations (Petrov and Petrova,⁽³⁾ Charlesworth,⁽²⁶⁾ Tomlinson, *et al.*⁽²⁷⁾ and Burrill, *et al.*⁽²⁹⁾)
- Deposit Thickness – 2 Models or Sets of Equations (Liebovitz⁽¹⁷⁾ and Tomlinson, *et al.*⁽²⁷⁾)
- Removal Rate – 2 Models or Sets of Equations (Voronov, *et al.*⁽¹⁶⁾ and Charlesworth⁽²⁶⁾)

Discussion

The following overlapping output parameters were found for soluble material:

- Hideout – 3 Models or Sets of Equations (Cleary, *et al.*,⁽⁵⁾ Millett and Fenton^(23,24) and Baum, *et al.*⁽²⁵⁾)
- Mass of Material Deposited – 3 Models or Sets of Equations (Mann and Castle,⁽¹⁵⁾ Cleary, *et al.*⁽⁵⁾ and Mizuno, *et al.*⁽³¹⁾)
- Concentration in Porous Media – 4 Models or Sets of Equations (Jones, *et al.*,^(18,19) Gonzales and Spekkens,⁽²²⁾ Ulke and Goldberg,⁽²¹⁾ and Millett and Fenton^(23,24))
- Deposition Rate – 2 Models or Sets of Equations (Mizuno, *et al.*⁽³¹⁾ and Bellows⁽³⁸⁾)

Probable areas were identified where the feasibility of interconnection between modules may be a problem because of missing data or models. The impact of this missing information on the success or enhancement of the comprehensive model was identified. Also, lack of available data or constants for application to fossil plants was identified. The assessment of the required input values was again based on the 1-4 ranking system:

- 4 – Parameter that is relatively well known
- 3 – Parameter that is possible to establish or define, but may not be well known
- 2 – Parameter that is more difficult to establish or define
- 1 – Parameter that may be very difficult to establish or define with known certainty

The results are given in Table 3-1. Again, some of the inputs were calculated from the output of complimentary equations (indicated as “calculated” in Table 3-1). The same value was used for ranking a specific parameter of soluble, insoluble or thermal-hydraulic input. Items with a relatively low ranking and a moderate to high importance may need to be better defined. Assumptions can be made in some cases until more data or measurements are available. These items are as given below:

- Deposit geometry – capillary length, chimney length, tortuosity, volume of pores, deposit porosity, deposit surface area (not flat), capillary cross-sectional area
- Deposit thermal conductivity, especially for layered deposits
- Concentrated liquids – Density and viscosity, if not available in the literature
- Thermal-hydraulic and chemistry coefficients – diffusion coefficient, mass transfer coefficient, deposition coefficient, re-entrainment coefficient, dissolution coefficient
- Single phase permeability

Of these items, the most significant at this time appears to be the deposit geometry.

Table 3-1
Ranking of Input Parameters

PARAMETER	RANKING VALUE	PARAMETERS USED IN EQUATIONS FOR INSOLUBLE MATERIALS	PARAMETERS USED IN EQUATIONS FOR SOLUBLE MATERIALS	PARAMETERS USED IN T/H FEEDBACK EQUATIONS	NOTES
TIME	4.0	X	X	X	
POWER	4.0	---	X	---	
BULK MASS/VOLUME	4.0	X	X	---	
BULK SUBCOOLING	4.0	---	X	---	
SURFACE TEMPERATURE	4.0	---	X	---	
BULK TEMPERATURE	4.0	X	X	X	
BULK PRESSURE	4.0	---	X	X	
VELOCITY	4.0	X	X	---	
FLOWRATE	4.0	X	X	---	
STEAM VISCOSITY	4.0	---	X	---	
STEAM DENSITY	4.0	---	X	---	
WATER DENSITY	4.0	X	X	---	
HEAT OF VAPORIZATION	4.0	X	X	---	
BULK CONTAMINANT CONCENTRATION	4.0	X	X	---	
BULK DEPOSITING CONCENTRATION	4.0	X	X	---	
BLOWDOWN RATE	4.0	X	X	---	
DIELECTRIC CONSTANT	4.0	X	---	---	
DEPOSITION RATE CONSTANT	3.5	---	X	---	a
DEPOSIT THICKNESS	3.5	X	X	X	a
DEPOSITION RATE	3.3	X	---	X	a
CONCENTRATION OF CONCENTRATED LIQUID	3.3	X	X	---	a
CONCENTRATION IN STEAM	3.4	X	X	---	a,b
DIFFUSION MASS TRANSFER	3.2	X	X	---	a
CONVECTION MASS TRANSFER	3.2	X	X	---	a
HEAT FLUX	3.0	X	X	---	
HYDRAULIC DIAMETER	3.0	---	X	---	
STEAM QUALITY	3.0	X	X	---	
PARTICLE SIZE (DIAMETER)	3.0	X	X	---	
SOLID PARTICLE DENSITY	3.0	X	---	---	
TOTAL MASS OF PARTICLES	3.0	X	X	---	
SUBSTRATE SURFACE AREA	3.0	X	X	---	
DEPOSIT COMPOSITION	3.0	---	X	X	
CHIMNEY POPULATION DENSITY	3.0	---	X	---	
FRACTION OF AREA W/O CHIMNEYS	3.0	---	X	---	
WETTED CHIMNEY LENGTH	3.0	---	X	---	
CHIMNEY CROSS-SECTIONAL AREA	3.0	---	X	---	
pH	3.0	X	X	---	
UNIT CHARGE	3.0	X	---	---	
MOLECULAR VOLUME	3.0	---	X	---	
DISTRIBUTION RATIO	3.0	---	X	---	
ACTIVITY COEFFICIENT	3.0	---	X	---	
DISSOCIATION CONSTANT	3.0	---	X	---	
SOLUBILITY CONSTANT	3.0	X	X	---	
HIDEOUT	3.0	---	X	---	
HIDEOUT RETURN	3.0	---	X	---	
SINGLE PHASE PERMEABILITY	2.7	---	X	---	a
HYDRATION NUMBER - WATER	2.7	---	X	---	a
LIQUID VISCOSITY	3.0	X	X	---	a,c
REGION-TO-REGION FLOWRATE	2.0	X	---	---	
SURFACE TENSION	2.0	---	X	---	
DEPOSIT SURFACE AREA	2.0	X	X	---	
NUMBER OF DEPOSITED PARTICLES	2.0	X	---	---	
DEPOSIT THERMAL CONDUCTIVITY	2.0	---	X	X	
CHIMNEY RADIUS	2.0	---	X	---	
DEPOSIT POROSITY	2.0	X	X	X	
CAPILLARY CROSS-SECTIONAL AREA	2.0	---	X	---	
STICKING FACTOR	2.0	X	---	---	
MASS TRANSFER COEFFICIENT	2.0	X	X	---	
DISSOLUTION COEFFICIENT	2.0	X	---	---	
DENSITY OF CONCENTRATED LIQUID	2.0	X	X	---	
CORROSION CURRENT DENSITY	2.0	X	X	---	
SURFACE POTENTIAL	2.0	X	---	---	
HYDRATION NUMBER - STEAM	2.0	---	X	---	
HAMAKER CONSTANT	2.0	X	---	---	
SEPARATION DISTANCE	1.0	X	---	---	
VOLUME OF PORES	1.0	---	X	---	
CAPILLARY LENGTH	1.0	---	X	---	
TOTAL CHIMNEY LENGTH	1.0	---	X	---	
TORTUOSITY	1.0	---	X	---	
DIFFUSION COEFFICIENT	1.0	X	X	---	
DEPOSITION COEFFICIENT	1.0	X	---	---	
RE-ENTRAINMENT COEFF & FACTOR	1.0	X	---	---	
GROWTH RATE COEFFICIENT	1.0	X	---	---	

(a) This parameter has a ranking value that was calculated using ranking of other input values..

(b) This parameter has a ranking value that ranges from 3.2-3.5. The average value is shown above.

(c) This parameter has a ranking value that ranges from 2.0 - 4.0. The average value is shown above.

Discussion

The results of this assessment indicate that an aggregate model can be derived that can describe deposition in fossil boilers and other components. This model would be based on simple geometrical configurations, such as cylindrical symmetry. The accuracy of application of such a model to specific localized geometry, where the simple symmetry does not apply, is uncertain. For example, small stepwise change in tubing diameter can be easily modeled. Weld beads, small welding supports and tube ribs or rifling may be more challenging to model. Local conditions in steam-water circulation circuits can produce localized deposits that are much more difficult to model. The input parameters, that describe the localized geometry of the component (such as local velocity, temperatures, heat flux, flow patterns, etc.), must be known in order for the model to produce the desired results. Additionally, the model equation may need to be altered for such local conditions. Nonetheless, the general aggregate deposition model must be designed before more local conditions can be modeled.

In general, the aggregate deposition model will consider many local conditions, such as boiling and depositing in steam chimneys. However, considerable knowledge of the physical characteristics of these deposits is required for the modeling. If the input parameters that describe the physical characteristics (porosity, tortuosity, etc.) of the deposits are not well characterized, the results may have significant errors. That is, if the input values do not describe the deposit characteristics, no model can produce the desired results.

3.3 Limitations of the Assessment

The following limitations apply to the methodology used for this assessment:

- The impact of a specific parameter may be larger than indicated by this linear assessment (for example, heat flux is treated equally with temperature although heat flux may be a second to fifth order contributor whereas temperature may be a linear contributor).
- Although the applicable range of each input and output parameter is noted in Section 2, if it was available in the original work, the ability to extrapolate the result of parameters that are not within the range of the fossil power plant application was not considered explicitly in the assessment in Section 3. This would require supplementary assessments that can only be done after portions of the aggregate model are constructed.
- The models and equations were not checked for accuracy.
- Steady-state and time dependent equations were treated equally (although this characteristic is noted in the text).
- The logic used by each author for solving the equations (for example, exact solution or iteration) was not checked and may differ among the various models using similar equations.
- The logic used to combine various input variables is very specific in each model, and the specificity was not analyzed, even if it can be derived from the text in Section 2.
- The definition of some parameters was not completely explained in all of the references. The assumption of identical parameters among two or more references may not be totally correct, depending on the details of the definitions. For example, “wetted length” and “tortuosity” may differ in understanding among various authors.

- The ability to combine equations from several investigators cannot be affirmed until the construction of the aggregate model is undertaken. The current assessment assumes that combining equations is possible if the input or intermediate output parameters appear to be compatible. For example, the synergy between soluble and insoluble materials was, in some cases, based on empirical coefficients or plant measurements. This may be better accomplished with the high-temperature solubility data available from other investigators, although data may not be available for all chemical species. However, no attempt was made under the current assessment to combine these equations.
- Although a large number of input parameters and coefficients were found, numerous other parameters were not considered, based on the priority established in earlier assessments.^(1,2)
- Each author elected to neglect some important parameters, as expected, based on the specific aspect of deposition that was considered important for the application or respective investigation. Some of these other parameters in the application or test may not have been controlled or analyzed by either the original authors or by this assessment. That is, unspecified parameters are assumed to be constant or not important.

3.4 Portions of Selected Models for Future Development

A combination of equations will be required to develop the aggregate model. The following modules will be required for future development of the aggregate model:

- High-temperature, high-pressure solubility of various chemicals in steam, such as that provided by Palmer, *et al.*⁽³²⁻³⁶⁾ to describe the chemicals that will be carried out of a porous deposit under local boiling conditions.
- High-temperature water solubility of various compounds, such as that provided by Palmer, *et al.*⁽³²⁻³⁶⁾ and Liebovitz,⁽¹⁷⁾ to describe the amount and concentration of chemicals that will remain in an aqueous, corrosive form, may deposit as solids and can densify the deposits (plugging the capillaries and chimneys). This will include hideout and hideout return considerations, such as those presented by Millett and Fenton.^(23,24)
- Continuity, momentum, energy (heat transfer), and mass transfer models, such as those provided by Jones, *et al.*,⁽¹⁸⁻¹⁹⁾ Petrov and Petrova⁽³⁾ and Matijevic, *et al.*,⁽⁷⁾ that describe the boiling and concentrating of chemicals in porous media for selected, localized geometries in boilers.
- Deposition and removal, such as those presented by Petrov and Petrova,⁽³⁾ Tomlinson, *et al.*⁽²⁷⁾ Mann and Castle,⁽⁴⁾ Beal and Chen,⁽⁸⁾ Charlesworth,⁽²⁶⁾ Turner,⁽³⁸⁾ Bellows⁽³⁸⁾ and Burrill.⁽²⁹⁾

The first version of the aggregate model would present symmetric coordinate formulas for application to very specific boiler geometries. Subsequent versions of the models for asymmetric localized conditions will need alternate limit conditions and/or alternate equations.

4

CONCLUSIONS AND RECOMMENDATIONS

The review of available models and equations, encompassing deposition of soluble and insoluble material on heat transfer surfaces, indicates that it is feasible to create an aggregate model for surfaces with symmetrical geometries. There is an abundance of usable first-principle equations that employ coefficients from experiments performed by several prominent authors (or in some cases borrowed from other authors). This makes a case for a high probability of success with an aggregate model for fossil plant boiler applications.

A total of 73 input parameters (including coefficients) and 26 intermediate and final output parameters were tabulated for the references that were assessed. This is higher than the approximately 40 parameters that were initially identified in the earlier state-of-knowledge investigation. However, the earlier investigation did not consider coefficients and other supplementary inputs. Furthermore, the actual number of input parameters required to exercise a specific calculation to produce a final result ranges from 1 – 22, depending on the selected calculation route. That is, the literature contains both simple and complex models that can be considered for incorporation into the aggregate model. A limited number of final output parameters were identified for the soluble and insoluble material, including deposition rate, deposit thickness, mass of material deposited, hideout and concentration in porous media. Adsorption was considered as a subset of soluble and insoluble deposition processes.

The input and output parameters were ranked on a scale of 1 – 4, based on an engineering judgment of the current state-of-knowledge of that parameter and a simple algorithm that related input and output parameters, as follows:

- 4 – Parameter that is relatively well known
- 3 – Parameter that is possible to establish or define, but may not be well known
- 2 – Parameter that is more difficult to establish or define
- 1 – Parameter that may be very difficult to establish or define with known certainty

The ranking of the final output parameters on the scale of 1 – 4 is as follows for insoluble material (metals and metal oxides):

- Mass of Material Deposited 3.0 (76%)
- Deposition Rate 3.3 (82%)
- Deposit Thickness 3.5 (86%)
- Removal Rate 3.2 (80%)

Conclusions and Recommendations

The ranking of the final output parameters on the scale of 1 – 4 is as follows for soluble material (sodium chloride, etc.):

- | | | |
|---------------------------------|-----|-------|
| • Hideout | 3.0 | (76%) |
| • Mass of Material Deposited | 3.6 | (90%) |
| • Concentration in Porous Media | 3.3 | (83%) |
| • Deposition Rate | 3.5 | (88%) |

Two to four overlapping sets of equations or models were found that describe the final output parameters, with additional overlap on the intermediate output. This overlap can be handled in the aggregate model during design of the model or, in some cases, allowed to become user selected options for specific applications.

A combination of the equations or models will be required to develop the aggregate model. The first version of the aggregate model would present symmetric coordinate formulas for application to very specific boiler geometries. Subsequent versions of the models for asymmetric localized conditions will need alternate limit conditions and/or alternate equations.

The aggregate model should consider initial deposition on a clean surface, followed by growth until maturing of the deposit, including boiling and deposition within capillaries and steam chimneys within the deposit. This process will require inputs for bulk and local thermal hydraulic conditions, as well as solubility information for pertinent chemicals in the bulk and local water and steam.

Considerable knowledge of the physical characteristics of these deposits is required for this type of modeling. If the input parameters, that describe the physical characteristics (porosity, tortuosity, etc.) of the deposits, are not well known, the results may have significant errors. That is, if the input values do not describe the deposit characteristics, no model can produce the desired results.

After the initial model is developed, it will probably be necessary to conduct laboratory experiments and/or plant measurements to benchmark the model and, in some cases, to obtain better coefficients for the model in general. This may be especially necessary for asymmetrical local geometries, such as weld beads, weld rings and tube ribs. As a first approach, these local conditions may be treated as a subset of the overall calculation to determine if the model adequately describes the deposition patterns. This is similar to the approach used by Jones, *et al.* ^(18,19) in modeling the deposition within porous deposits. However, some local conditions may require additional subroutines within the model to adequately describe these cases. This should not hamper the initial development of an aggregate model.

The model is only as good as its coefficients. Investigators have shown cases in which the experimental (or plant) results can be 10-100x different from those predicted by a first-principle model (including experimental coefficients). Also, combining several models, each of which has experimental coefficients into an aggregate model may compound the error.

Many of the existing models have been generated in response to the needs of the nuclear industry, including heat transfer from zirconium alloy nuclear fuel rods and through nickel alloy steam generator tubes. However, the heat flux is largely similar to that of boilers in fossil plants, although temperature and pressure are lower. Chemistry and deposit composition, as well as local geometric conditions, may also differ.

The following steps will be required for development of an aggregate model that is applicable to fossil plant boilers:

1. Equation List – Prepare a list of all required equations in common terms and common units based on the input parameters required to produce the following output parameters:
 - Mass of material deposited and hideout
 - Deposition rate
 - Deposit thickness
 - Removal rate
 - Concentration in porous media
2. Solutions – Develop solutions for the differential equations, explicitly or numerically, for steady state and, if necessary, transient conditions.
3. Estimate – Estimate initial values for input parameters and coefficients that are not known precisely for fossil power plants, based on available information for other applications. This may include the following input parameters (including coefficients) for the geometries of interest in boilers and turbines:
 - Deposit geometry – capillary length, chimney length, tortuosity, volume of pores, deposit porosity, deposit surface area (not flat), capillary cross-sectional area
 - Deposit thermal conductivity, especially for layered deposits
 - Concentrated liquids – Density and viscosity, if not available in the literature
 - Thermal-hydraulic and chemistry coefficients – diffusion coefficient, mass transfer coefficient, deposition coefficient, re-entrainment coefficient, dissolution coefficient
 - Single phase permeability
4. Preliminary Model – Develop a preliminary model based on estimated input parameters. This model may consist of spreadsheets or other means for use in understanding the interactions of the various equations.
5. Platform – Select a computer software platform and programming interface with software used by major equipment suppliers/owners.
6. Programming – Write the software necessary to solve the equations and satisfy the interactions with computer codes of major equipment suppliers.

Conclusions and Recommendations

7. Document And Test Software – Document the software and perform the necessary quality control tests to assure that the software is functioning correctly with the best available values for input parameters and coefficients.

The following steps will be required in support of the model development:

1. Physical Measurements – Prioritize and make physical measurements of the following input parameters for the geometries of interest in boilers and turbines, as necessary, to support the initial estimates of input parameters and coefficients, such as deposit geometry, thermal conductivity, concentrated liquids, thermal-hydraulic coefficients, chemistry coefficients and single phase permeability. Of these items, the most significant, at this time, appears to be the deposit geometry. The activity may be performed in connection with or as a result of information gained from benchmarking and laboratory testing.
2. Benchmarking – Establish methods to benchmark and identify deficiencies in the aggregate model, including possible comparison of deposition patterns in operating fossil plants. Special attention should be given to asymmetrical local geometries, such as weld beads, weld rings and tube ribs.
3. Laboratory Testing – Perform additional laboratory tests to obtain the required information for any deficiencies identified by the benchmarking. The additional information may include updated input parameters, coefficients or new equations and subroutines.
4. Code Revision – Revise the computer code to include updated values for input parameters, coefficients and equations, based on additional laboratory data and physical measurements. Document and test the revisions.

5

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A

COLLOQUIUM ON MODELING DEPOSITION IN FOSSIL FUEL PLANTS

A Colloquium on Modeling Deposition in Boilers of Fossil Fueled Power Plants was held on January 28 - 29, 2004 at the Electric Power Research Institute (EPRI) office in Charlotte, NC. A select group of experts with knowledge of the subject were invited to attend. Those in attendance were, as follows:

Bill Allmon, Framatome ANP, Inc.

Jim Bellows, Siemens Westinghouse Power Corporation

Barry Dooley, EPRI

Steve Goodstine, Alstom Power Inc

Barclay Jones, University of Illinois at Urbana-Champaign

Lee Machemer, Jonas, Inc.

Don Palmer, Oak Ridge National Laboratory (ORNL)

Mike Pop, Framatome ANP, Inc.

Andrei Petrov, Moscow Electric Power Institute (MPEI)

Tamara Petrova, Moscow Electric Power Institute (MPEI)

Kevin Shields, EPRI

Carl Turner, Atomic Energy of Canada (AECL), Chalk River Laboratories

The Colloquium provided an excellent exchange of ideas and discussion of possible ways to connect existing knowledge, equations and models into a comprehensive aggregate model for fossil plant cycles. Highlights are as follows:

- More data needs to be obtained on the morphology of deposits in fossil boilers and on hydrogen damage mechanisms in Heat Recovery Steam Generators (HRSG).
- Recommendations on flow dynamics and circulation ratio need to result from model usage.
- One significant endpoint of the modeling effort would be a prediction of when to chemically clean fossil boilers. A useful contribution of the model would be the capability to predict the amount of deposition around flow disruptions.
- Simple, affordable monitoring is needed to measure the need to chemically clean.

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- Several presentations contained examples of successful first, principle models that were simple. These models did not contain extensive equations with elaborate solutions.
- Model development should contain comparisons with experimental and/or field data that are as close to the modeled phenomena as possible.
- Model development should be done in a step-wise manner to allow early success, continued improvement and expansion into additional parts of the cycle.
- Model development should begin with the components that are most likely to encounter deposition-related corrosion and performance degradation. The two targeted components should be the boiler and turbine.
- With regard to boiler waterwall surfaces, model development should consider individual plant types and possible step-wise model development according to plant type, categorized as follows:

Subcritical plants with boiler tube failures (BTF),

Subcritical plants without BTF,

Supercritical plants with oxidizing chemistry and, possibly,

Supercritical plants with reducing chemistry.

- A review of the Russian deposition data and models for boiler deposition were presented by Tamara Petrova of the Moscow Electric Power Institute. Ten major contributors to deposition were described including (1) heat flux, (2) heat transfer condition, (3) enthalpy, (4) concentration of corrosion products, (5) fluid temperature, (6) pH, (7) water chemistry, (8) composition of water impurities and (9) period of operation. Heat flux was described as having a second order impact on deposition rate; heat flux also has a role in electrokinetic deposition. Concentration was shown to have a linear impact on deposition. Solution pH impacts both the isoelectric point and solubility. Large amounts of data were available for this review, but some researchers had not completely described the test conditions. Most tests were conducted with high iron concentrations.
- Developments in chimney evaporation phenomena and solubility problems associated with chimneys were presented by Mike Pop from Framatome ANP and Barclay Jones of the University of Illinois. Modified wick boiling models were described for capillaries and chimneys in porous deposits on heat transfer surfaces. Deposition from soluble and insoluble material was described for various boiling regimes. Deposition and re-entrainment of insoluble material were considered. The impact of Van de Waals and electrical double layer (EDL) were included in deposition. EDL depends on pH, temperature, heat flux, velocity and other parameters. Deposition showed a linear dependence on velocity of the two phase flow and steam quality. Results were presented on the impact of subcooled boiling, wall superheat, deposit porosity, deposit thickness and heat transfer mode.
- Developments in databases on solubility were described by Don Palmer of Oak Ridge National Laboratory. Laboratory results on the solubility of nickel oxides, nickel hydroxides, copper oxides and other metal oxide/hydroxides in water were presented as a function of pH and temperature. Laboratory results were shown for the solubility of sodium chloride and copper oxides in steam. Additionally, laboratory results for the absorption of metal ions on

metal oxides were presented showing the absorption of nickel ion on titanium dioxide at various pH's. The pH was shown to have a significant impact (nine orders of magnitude change for nickel with pH change from 5 to 10). Finally, a presentation was made on the electrical double layer (EDL) modeling for titanium dioxide water interface.

- A model for deposition associated with forced convection and film boiling was presented by Carl Turner of Atomic Energy of Canada Limited (AECL). The model is empirical and is based on experimental results with synthetic corrosion products containing ^{59}Fe radiotracers. Synthetic corrosion products included colloidal magnetite, hematite and lepidocrocite and in-situ prepared ferrous precipitates. Testing considered fouling and removal, as monitored by changes in radioactivity, over a period of about 100 hours. The testing consisted of a series of heated and unheated test sections encompassing subcooled water to 60% steam quality. The tests considered the impact of chemical additives. The computer code calculates single-phase and two-phase deposition in a 3D mesh with several thousand nodes. The code calculates fouling on tubes and horizontal surfaces. Consideration is given to temperature, flow rate, heat transfer regime, heat flux, steam quality, flow pattern, fouling geometry, electrically charged interfaces and dispersion of corrosion products.
- Lee Machemer of Jonas, Inc. presented data and experiments on (a) surface adsorption or absorption of ionic material on metal oxides, (b) colloidal deposition and (c) orifice deposition and recommendations for model development. The development should produce a practical model based on field observations, laboratory data and theory. Theory should include thermodynamics, flow, surface phenomena and sources and transport of particles. The model should cover normal operation, transients, hydrostatic testing, cleaning, storage and shop practices. Combined cycles and older units should be considered. Consideration should be given to the roles of velocity; Reynolds number; boundary layer; gravitational forces; boiling; heat flux; water chemistry, including dispersants; surface adsorption or absorption; surface morphology; suspended and colloidal oxides, including nickel and zinc; crystal growth; zeta potential; contaminants, including organics; dynamics of deposition and release, pre-operational and operational cleanings; sampling and steam and air blow.
- A model for deposition of soluble material in turbines was presented by Jim Bellows of Siemens Westinghouse. The model is applicable to subcritical and supercritical turbines, and the principles are likely applicable to single phase deposition in other parts of the cycle. The turbine model considered deposition from single-, dry-phase steam. Deposition from single-phase water would use many of the same equations, according to the author. The turbine model did not consider two-phase water/steam conditions. The model includes solubility, homogeneous nucleation, heterogeneous nucleation and mass transfer. The model included no adjustable parameters. Examples of the model application were shown for deposition of silica and sodium chloride. Deposition appears to be more rapid than removal. Preliminary results indicated a significant impact at low load.
- Deposition in operating fossil boilers and design considerations for deposition in boilers were described by Steve Goodstine, Alstom Power. Boiler designs contain an engineering margin; however, no specific allowance is made for internal boiler tube deposition. Typical wall temperatures were shown, with and without deposits, for gas temperatures $>1,535^{\circ}\text{C}$ ($>2,800^{\circ}\text{F}$) and heat flux of 315 kW/m^2 (10^5 BTU/hr-ft^2). Examples of deposit-related failures and chemical cleaning solutions were shown. External corrosion fatigue may be

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related to internal deposits (deposition on the hot side of a tube contributes to expansion and bowing). Deposits can be layered 0.50-0.75 mm (20 -30 mils). Concentrating in films and porous deposits was described. Previous testing in a 3 MW test heat transfer and corrosion test loop was described. The 6-m (20-ft) test sections in the loop were electrically heated ($180^{\circ}/360^{\circ}$), and synthetic precipitated iron oxide was added to achieve deposition. Although the test loop has been dismantled, some of the data may be applicable to the modeling effort. Tests were conducted for ASME (1960's), rifled tubing (1980's) and phosphate (EPRI, 1990's). Field problems appear to have a degree of randomness, and minor variations appear to have significant effects. Prediction of orifice fouling would be beneficial.

Four questions were addressed by the attendees on the second day of the meeting:

1. Do you have a model (theoretical or empirical), data or analysis to recommend for inclusion in the aggregate model for fossil boilers, turbines or BOP?
2. Do you know of models (within your organization or otherwise) that you recommend should be considered for inclusion in the aggregate model for fossil boilers, turbines or BOP?
3. What are the perceived impediments to developing the aggregate model and/or in applying your model to the aggregate model for fossil boilers, turbines or BOP?
4. Does your recommended model, data or analysis address deposition in (a) subcritical plants with boiler tube failures (BTF), (b) subcritical plants without BTF, (c) supercritical plants with oxidizing chemistry and/or (d) supercritical plants with reducing chemistry?

The responses are summarized in Tables A-1 – A-7 in terms of deposition of particulate or soluble material and surface phenomena, as described below:

- Particles – Attachment/deposition of colloidal particles to surfaces
- Soluble – Formation of deposits from low solubility materials
- Surface Phenomena – Adsorption, absorption and/or ion exchange on surfaces of particulate materials

Highlights were as follows:

- Availability of Equations, Model or Data – Nearly all of the presenters had equations and/or models that may be directly or indirectly applied to the aggregate model, including a turbine model. The models were theoretical and empirical and concentrated on particulate deposition, except the turbine model, which concentrated on dissolved species. The remaining presenters had data that may be useful in developing and/or benchmarking the aggregate model. Some data would need to be correlated.
- Other Models – The presenters indicated other deposition equations and models in the literature that compliment their work.
- Impediments to Development of Aggregate Model – Missing data and the potential complexity of an aggregate model were seen as impediments. Also, detailed thermal-

hydraulic performance models, necessary for modeling the local deposition phenomena, may be proprietary.

- Type of Plant and Part of Cycle Addressed – The boiler models and equations are primarily applicable to subcritical units. The turbine model is applicable to subcritical and supercritical units.

Table A-1
Summary of Comments And Recommendations From Siemens Westinghouse

DEPOSITION TYPE	PARTICULATE	SOLUBLE	SURFACE PHENOMENA
Description of Your Model, Data or Analysis	Possibly	Yes	No
Other Models or Data of Interest		Yes	No
Perceived Impediments	Need for accurate parameters Molecular modeling Some direct measurements Need for validation Field measurements Comparison with converging-diverging nozzle data		
Application of Model to Boilers, Turbines or BOP*	Turbines - A*, B*, C* and D* And Principles Apply to Boilers, Also	Turbines - A*, B*, C* and D* And Principles Apply to Boilers, Also	
Comments	Field data Morphology of turbine deposits, particularly iron deposits Chemical and steam condition history between inspections	Field data Quantitative deposit data Methods need to be developed Chemical and steam condition history between inspections	
Presenter	James C. Bellows, Siemens Westinghouse Power Corp		

* Application Categories

A* = Subcritical Deposition With BTF

B* = Subcritical Deposition Without BTF

C* = Supercritical Deposition – Oxidizing

D* = Supercritical Deposition – Reducing

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Table A-2
Summary of Comments and Recommendations from Atomic Energy of Canada Limited

DEPOSITION TYPE	PARTICULATE	SOLUBLE	SURFACE PHENOMENA
Description of Your Model, Data or Analysis	Fouling Under Flow Boiling Conditions: <u>Model</u> A. Applicable to Normal Deposit Growth in Non-Disrupted Flow B. Model Does Not Account for Disrupted Flow Effects C. Rate Constants from Loops Tests on: • Deposition (Transport Plus Attachment) • Removal • Consolidation • Effect of Chemistry (pH, Amines, Dispersants and Surfactants) <u>Empirical Data</u> A. Loop Data Published in Appendices to EPRI Reports	None	None
Mechanism	(1) Forced Convection (2) Film Boiling		
Other Models or Data of Interest	AECL Model of Measured of Deposit Thermal Resistance Published		
Perceived Impediments	A. Modifications Needed to Make Model Applicable to Fossil Boilers and BOP B. Does Not Model Aerosol Deposition		
Application of Model to Boilers, Turbines or BOP*	A* and B* Not C* and D* Not Applicable to Turbines		
Comments	Particle Flow Under Flow Boiling Conditions Is For Nuclear OTSG and RSG Total Fouling Equals Forced Convective Plus Boiling Suggestions: A. Flow Regimes and Modes of Heat Transfer are Very Important B. Role of pH and Additive on Particle Trapping in Bubbles Is Very Important C. Investigate Effect of Flow Disruption on Fouling		
Presenter	Carl W. Turner, Atomic Energy of Canada Limited		

* Application Categories

A* = Subcritical Deposition With BTF

B* = Subcritical Deposition Without BTF

C* = Supercritical Deposition – Oxidizing

D* = Supercritical Deposition – Reducing

Table A-3
Summary of Comments and Recommendations from University of Illinois

DEPOSITION TYPE	PARTICULATE	SOLUBLE	SURFACE PHENOMENA
Description of Your Model, Data or Analysis	Deposition on Clean Surface with Boiling Porous Layer Performance (Chimney Model) With: • Physical Structure • Thermal Conditions • Concentration of Oxidizing/Reducing Chemicals	Solute Concentration on Clean Surfaces	
Mechanism			
Other Models or Data of Interest	A. Boiling Model of Surface Abnormalities B. Initial Work on at University of Illinois on Molecular Dynamics Modeling		
Perceived Impediments	A. Few Experiments Available to Validate Modeling for Surface Abnormalities B. Few Experiments Available to Validate Modeling on Molecular Dynamics		
Application of Model to Boilers, Turbines or BOP*			
Comments	Broad Application		
Presenter	Barclay G. Jones, University of Illinois at Urbana-Champaign		

* Application Categories

A* = Subcritical Deposition With BTF

B* = Subcritical Deposition Without BTF

C* = Supercritical Deposition – Oxidizing

D* = Supercritical Deposition – Reducing

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Table A-4
Summary of Comments and Recommendations from Moscow Electric Power Institute

DEPOSITION TYPE	PARTICULATE	SOLUBLE	SURFACE PHENOMENA
Description of Your Model, Data or Analysis	Equations Presented By MPI Could Be Used for Description of Deposition Processes		
Mechanism			
Other Models or Data of Interest	More Deposition Models Available in Literature		
Perceived Impediments	Define a Critical Location for Which the Model is Paramount Importance		
Application of Model to Boilers, Turbines or BOP*	A*, B*		
Comments	A. Development Should Move from a Simple to More Extensive Model Trying to Define Relative Influence of Parameters B. Model Should Address Local Flow Disruptions C. Ideally the Model Should Be Generic, But in Practice This Is Impossible to Achieve - So, It Will Be A Combination of Generic and Empirical D. Use of Model Boiler Data is Paramount to Verify Different Types of Local Disruptions E. It Would Be Very Desirable to Have Fully Instrumented Field Boiler to Verify Models		
Presenter	Tamara Petrova, Moscow Electric Power Institute, and Andrei Petrov, Moscow Electric Power Institute and Oak Ridge National Laboratory		

* Application Categories

A* = Subcritical Deposition With BTF

B* = Subcritical Deposition Without BTF

C* = Supercritical Deposition – Oxidizing

D* = Supercritical Deposition – Reducing

Table A-5
Summary of Comments and Recommendations from Oak Ridge National Laboratory

DEPOSITION TYPE	PARTICULATE	SOLUBLE	SURFACE PHENOMENA
Description of Your Model, Data or Analysis		Experimental Data on Solubility of AlOOH , NiO , ZnO , Zn/Co Chromites, Magnetite, Hematite, Copper Oxides and Ferrites	Adsorption at Temperature Greater Than 100°C (212°F) on Magnetite and ZrO_2 (Function of pH)
Mechanisms		Dissolution in Water	Adsorption
Other Models or Data of Interest		Model (OLI) and Other Supporting Models (EQ 3/6, CHILLER and ASPEN)	
Perceived Impediments		Data Selection Process - Interface Between Field Data and Basic Science - Identify and Fill Data Gaps Resulting from Extrapolation – Requires New Experiments	No Data on Hematite
Application of Model to Boilers, Turbines or BOP*		A* and B* Very Little C* and D* Data	
Comments			
Presenter	Donald A. Palmer, Oak Ridge National Laboratory		

* Application Categories

A* = Subcritical Deposition With BTF

B* = Subcritical Deposition Without BTF

C* = Supercritical Deposition – Oxidizing

D* = Supercritical Deposition – Reducing

Colloquium on Modeling Deposition in Fossil Fuel Plants

Table A-6
Summary of Comments and Recommendations from Alstom Power

DEPOSITION TYPE	PARTICULATE	SOLUBLE	SURFACE PHENOMENA
Description of Your Model, Data or Analysis	No Deposition Models to Offer Potential T/H Codes or Output from T/H Codes	No Deposition Models to Offer	No Deposition Models to Offer
Mechanisms			
Other Models or Data of Interest	No Deposition Models to Offer	No Deposition Models to Offer	No Deposition Models to Offer
Perceived Impediments	View the Overall Program as Diverse and Complex with Different Environments and Conditions		
Application of Model to Boilers, Turbines or BOP*	No Comments	No Comments	No Comments
Comments	A. Support the Stage-Phased Approach Presented by Barry Dooley B. Include Turbine Deposition Early • Simpler • Important Driver for Feedwater Chemistry Limits C. Like Idea of Looking for Evidence in Field Samples to Support Models – Samples are Rarely Analyzed in Detail Sufficiently Early		
Presenter	Stephen L. Goodstine, Alstom Power		

* Application Categories

A* = Subcritical Deposition With BTF

B* = Subcritical Deposition Without BTF

C* = Supercritical Deposition – Oxidizing

D* = Supercritical Deposition – Reducing

Table A-7
Summary of Comments and Recommendations from Jonas, Inc.

DEPOSITION TYPE	PARTICULATE	SOLUBLE	SURFACE PHENOMENA
Description of Your Model, Data or Analysis	No Models to Offer Have Experimental and Field Data	No Models to Offer Have Experimental and Field Data	No Models to Offer Have Experimental and Field Data
Mechanisms	N/A	N/A	N/A
Other Models or Data of Interest	N/A	N/A	N/A
Perceived Impediments	The Model Should Provide Root Causes for Deposition and Recommendations on Reduction of Deposition (For Example, Design, Chemistry, Operation and Layup)		
Application of Model to Boilers, Turbines or BOP*	N/A	N/A	N/A
Comments	A. Model Should Go Beyond Steady State Conditions (Startup/ Layup) B. Model Should be Based on a Combination of Field Data, Chemistry (Thermal Sorption and Crystal Growth) and Flow Phenomena C. Model Should Also Account for Surface Finish (Original and After Deposition)		
Presenter	Lee Machemer, Jonas, Inc.		

* Application Categories

A* = Subcritical Deposition With BTF

B* = Subcritical Deposition Without BTF

C* = Supercritical Deposition – Oxidizing

D* = Supercritical Deposition – Reducing

B

EQUATIONS DESCRIBING SELECTED INDIVIDUAL PHENOMENA ENCOUNTERED IN DEPOSITS

This appendix contains pertinent groups of equations from a much larger set of equations presented in the unpublished work of Warwood, Roe and Sears,⁽³⁹⁾ including a listing of the input and output parameters and a general description of the equations. The reader is directed to the description of the degree by which power plant operational parameters influence the outcome of the process described by the equation.

B.1 Change of State, Thermodynamic Changes in Deposited Materials and Changes of Crystals in Deposits

MECHANISM	INPUT AND OUTPUT PARAMETERS	DESCRIPTION
Vapor/liquid equilibria	OUTPUT: L_i =mean potential energy difference per mole INPUT: n_v and n_L = number of moles per unit volume of vapor and liquid, respectively; R=gas constant; T=absolute temperature	The pressure at which a liquid and gas coexist in equilibrium is the saturation vapor pressure of the liquid at the given temperature. At each temperature selected, equilibrium will be attained when the number of molecules leaving the liquid is equal to the number returning in a given time. Only molecules possessing sufficient energy are able to vaporize. As the temperature is raised, the ratio $\frac{n_v}{n_L}$ increases, and since n_L does not vary appreciably with temperature, the molecular concentration in the gas phase, and therefore the vapor pressure, increases. Operational parameters influence the temperature and pressure of the system, and therefore the vapor pressure and distribution of liquid to vapor.
Thermodynamic equations of state for a closed system	OUTPUT: $(\frac{\partial S}{\partial V})_T$ Where S=entropy INPUT: P=pressure; V=volume; T=temperature	The vapor pressure, p, is dependent of the temperature but is independent of the volume of the liquid and vapor; therefore, dp/dT can replace $(\frac{\partial P}{\partial T})_v$. Operational controls will influence the temperature, system pressure, and concentration of suspended species, and therefore, the vapor pressure of the deposition materials.

Equations Describing Selected Individual Phenomena Encountered in Deposits

MECHANISM	INPUT AND OUTPUT PARAMETERS	DESCRIPTION
Thermodynamic equation of state for reversible heat uptake	OUTPUT: ΔS =change in entropy INPUT: ΔH =heat of evaporation (enthalpy); T=temperature	The increase in the heat content ΔH , is equal to the heat associated with the reversible process of evaporation. Operational parameters will influence the temperature and the pressure at which the change of state occurs.
Clausius-Clapeyron equation applied to liquid/gas transition	OUTPUT: $\frac{dp}{dT}$ Where p=vapor pressure INPUT: T=temperature; INPUT: ΔH =heat of evaporation; ΔV = increase in volume accompanying the vaporization of liquid	Since ΔV is the increase of volume associated with the vaporization of liquid, then $\Delta S / \Delta V$ has a constant value at each temperature and may be substituted for $((\frac{\partial S}{\partial V})_T$. The result is the relationship deduced by Clausius and Clapeyron. Operational parameters will influence the temperature and pressure of the system (which in turn affect the molar volume).
Clausius-Clapeyron equation for the crystal melting (fusion) process.	OUTPUT: $\frac{dT}{dP}$ Where T=temperature; P=total pressure INPUT: V_L, V_S =molar volumes of pure substance liquid and solid, respectively; L_f =molar latent heat of fusion	Crystal melting of a pure material occurs at a definite temperature, depending on the pressure of the system. As with evaporation and sublimation, the process of diffusion or melting is accompanied by an absorption of heat (i.e. latent heat of fusion). Since the volume change from liquid to solid is negligible, the internal latent heat differs very little from the total value measured at constant pressure. As a general rule, high pressures are required to produce an appreciable change of melting point. Operational parameters will influence the pressure and temperature of change of state.
Latent heat thermodynamic conservation	OUTPUT: L_S (Molar latent heat of sublimation) INPUT: L_f, L_e =molar latent heat of fusion, and evaporation, respectively	Since the same amount of heat must be absorbed in the conversion of a given quantity of solid directly to the vapor (L_S) as would be required for the change in two stages, first from solid to liquid (L_f) and then from liquid to vapor (L_e) , at the same temperature and pressure. Operational parameters will influence the temperature and pressure of the change of state.

Equations Describing Selected Individual Phenomena Encountered in Deposits

MECHANISM	INPUT AND OUTPUT PARAMETERS	DESCRIPTION
Modified Kirchhoff equation	OUTPUT: $\frac{dL_f}{dT}$ INPUT: C_L, C_S = molar heat capacities of liquid and solid, respectively; L_f = latent heat of fusion; T = temperature	The influence of temperature on the latent heat of fusion is often expressed by a form of the modified Kirchhoff equation. Since the melting point changes with applied pressure, so also will the latent heat; the direction of the change will depend on the sign of dT/dP . Operational parameters will influence the temperature and pressure of the change of state.
Clausius-Clapeyron equation for polymorphic change of crystalline structure	OUTPUT: $\frac{dT}{dP}$ Where T = temperature; P = pressure INPUT: V_α, V_β = specific volumes of the two crystalline forms, α and β , respectively; L_t = latent heat of transition per mole	Under certain conditions polymorphic substances have a transition point at which the two crystalline forms can coexist in equilibrium, whereas above or below this temperature only one of the forms is stable. There is only one temperature, at each pressure, at which the two crystalline forms can coexist, and so on heating or cooling the system must remain at the transition temperature while one form is changing into the other. Operational parameters will influence the temperature and pressure of the system, and the crystal constituents present.
Thermodynamic solubility product, K_a for precipitation equilibrium reaction at constant temperature.	OUTPUT: Thermodynamic solubility product K_a of the reaction of a solid electrolyte M_xA_y at constant temperature in water INPUT: a - the activity of the designated chemical species; x = no. of moles of cation M, with charge Z^+ ; y = no. of moles anion A, with charge b = no. of water molecules associated with M^{Z+} in solution; c = no. of water molecules associated with A^{Z-} in solution	Thermodynamic solubility product for a solid electrolyte, M_xA_y , in equilibrium with its saturated solution at constant temperature was derived from the law of mass action and gives the condition of equilibrium of a reversible chemical reaction. Operational control will influence the temperature of the reaction, the solutes involved in the precipitation reaction and any competing reactions.
Thermodynamic solubility product with constant solid phase activity and insignificant hydration effect on the activity of water.	OUTPUT: K_{SO} - Thermodynamic solubility product with constant solid phase activity and insignificant hydration effect INPUT: a - the activity of the designated chemical species; x = no. of moles of cation M, part of the solid electrolyte M_xA_y in water; y = no. of moles anion A, part of the solid electrolyte M_xA_y in water	Solubility product is defined for the equilibrium reaction of solid electrolyte M_xA_y in water, assuming the activity of the solid phase is constant and the hydration of ions has an insignificant effect on the activity of the water. Operational control will influence the temperature of the reaction, the solutes involved in the precipitation reaction and any competing reactions.

Equations Describing Selected Individual Phenomena Encountered in Deposits

MECHANISM	INPUT AND OUTPUT PARAMETERS	DESCRIPTION
Diffusion-controlled crystal growth	$\frac{dc}{dt} = kS(C - C_o)$ OUTPUT: dc/dt=rate of crystal growth INPUT: S=crystal surface area; k=transport coefficient (convection and diffusion); C_o=concentration of reactant at the crystal surface; C=concentration of reactant in the bulk solution	Growth of crystals involves transport of solute to the crystal/solution interlace, adsorption of the solute at the surface, and incorporation of the crystal constituents into the lattice. Rate of formation may be limited by the diffusion to the surface, rate of adsorption, or the rate incorporation. From a mechanistic viewpoint, the free energy of ion adsorption onto a crystal should be lowered by more contact with the surface. Therefore, the rate-limiting step in interlace-controlled crystal growth should be the adsorption of the first ion on a flat surface. Operational control will influence the surface reactivity (materials), concentration of solute material in the bulk solution, and temperature. Specific adsorption of ions on surfaces involves the formation of relatively strong chemical bonds similar to those occurring in precipitates. The fact that an ion is specifically adsorbed on the surface of a substrate suggests that it has a tendency to form an insoluble compound or stable complex with the ion of opposite charge in the substrate, or with other bound ions of the opposite charge.
Reaction rate constant for the precipitation or crystallization of a solid from a vapor	OUTPUT: K_{T_s}=reaction rate for the reaction occurring at T_s INPUT: p_i=partial pressure of component I; x, y, z=molar ratio of reaction: $A_{(s)} + xB_{(g)} \rightleftharpoons yC_{(g)} + zD_{(g)}$ where the forward reaction occurs at T_s, and the reverse reaction at T_D	For the reversible chemical reaction described, the reaction direction is preferential based on the temperature. At the temperature of T_s, the forward reaction is dominant (sublimation), whereas at the temperature T_D, the reverse reaction is dominant (deposition). Both reactions can occur simultaneously in a system where the reactant source (such as a suspended particulate containing precipitated or adsorbed material in suspension) is in the bulk carrier stream and the deposition site (piping system surfaces) is at a lower temperature of T_D. Operational parameters will influence the temperature of the source materials (bulk suspended particulate temperatures, boiler temperatures, superheater temperatures) and the deposition site temperatures (wall and surface temperatures). In addition, the concentration (partial pressure of reactants) will influence the reaction rates.
Supersaturation transport-at crystal face limited regime	OUTPUT: α=supersaturation INPUT: d=dilution factor due to the carrier gas steam pressure; K_{T_s}=reaction rate constant for the reaction proffered at T_s; K_{T_D}=reaction rate constant for the reaction preferred at T_D	This equation indicates that supersaturation and, therefore, the crystal growth rate is directly proportional to the source/substrate temperature ratio. Operational controls will influence the temperature of the source material, the substrate temperature, and the partial pressures of the reactant species.

Equations Describing Selected Individual Phenomena Encountered in Deposits

MECHANISM	INPUT AND OUTPUT PARAMETERS	DESCRIPTION
Tammann temperature	$T_{\text{Tammann}} = 0.5 T_{\text{melting point}}$ OUTPUT: T_{Tammann} Tammann temperature INPUT: $T_{\text{melting point}}$ Melting Temperature	The Tammann temperature and above is the temperature at which both ions and electrons are mobile from occupied sites to vacancies within the lattice during crystal formation. This “rolling” process is actually allowing re-arrangement of the ions within the amorphous solid into crystalline structures.
Born repulsion energy of ions in a crystal lattice.	OUTPUT: V_B = Born repulsive interaction energy for ions in a lattice INPUT: A = Madelung’s constant for the crystal (sum of the mutual potential energies of all the ions in the lattice; α = largest common factor in the valences of the ions; e = electronic charge; r_0 = equilibrium distance between ions when the potential energy for the lattice is at a minimum; n = number of molecules per unit cell in the lattice; x = compressibility factor of the crystal	The Born repulsive interaction energy for ions in the lattice is determined by evaluating it at the equilibrium distance of r_0 , when the potential energy per unit cell (ϕ) is at minimum. At $r = r_0$, $d\phi/dr = \text{zero}$, and the equation described results from the Born and Lande’ approximation. The compressibility of the crystal (x) for alkali halides varies generally from 6 to 10. The resulting repulsive energy term falls off very quickly with increasing distance. Operational controls will influence the ion concentration and the potential energy of the lattice compared to the dispersed ions in the system under the temperature, pressure, and concentration at operational conditions.

B.2 Dilute Solutions (Solvent - Solute Equations)

MECHANISM	INPUT AND OUTPUT PARAMETERS	DESCRIPTION
Vapor pressure of pure solvent and in solutions	OUTPUT: $\frac{d \ln(p / p^0)}{dT}$ Where p^0, p = vapor pressure of the solvent in a pure solvent and mixture, respectively INPUT: T=temperature; R=gas constant; L_e^0, L_e are the latent heats of vaporization of pure solvent and solvent from solution, respectively	The Clausius-Claperyon equation, in the form applicable to the liquid-vapor system with ideal gas behavior, can describe the effect of a solute on the vapor pressure of the solvent. Subtraction of the two equations describing the pure solvent and solution vapor pressures will result in the third equation for the change in vapor pressure for a solution from that of the pure solvent. Operational parameters will influence the temperature, pressure, and concentration of suspended species in the solution.
Raoult's law	OUTPUT: p = partial pressure of solvent in solution. INPUT: n_1, n_2 = moles of solvent and solute, respectively; x_2 = mole fraction of solute; p^0 = partial pressure of pure solvent	This equation, a form of Raoult's law, holds for ideal solutions. It states that the change in the number of moles of solvent and solute is reflected by the change in partial pressure of pure solvent and solute in solution. Operational parameters will influence the temperature, pressure, and concentration of solute in solvent for the solution.

B.3 Transport and Diffusion in Steam and Within Deposits

MECHANISM	INPUT AND OUTPUT PARAMETERS	DESCRIPTION
Linear Diffusion of a binary solution of component A diffusing in component B (Fick's first Law)	OUTPUT: J_{OA} = diffusion flux INPUT: D_{AB} = diffusivity of A into B; c_A = Concentration of A; $\frac{dc_A}{dx}$ = molar concentration gradient; $(u_A - u_0)$ = velocity component of A relative to the volume-average velocity (u_0)	This relationship is an example of Fick's first law expressed in terms of a molar flux. The implied direction of the chemical gradient driving force is perpendicular to the interface between the species. Steady state is assumed when the concentration at any point does not change with time. Operational procedures will affect the stagnant boundary layer thickness and density near surfaces, which will affect the diffusion velocities and the concentration gradient.
Fick's first law of diffusion based on gas partial pressures.	OUTPUT: $\frac{dc_A}{dx}$ - partial molar concentration gradient in the X direction INPUT: p_A = partial pressure of A; R = gas constant; T = absolute temperature; $\frac{dp_A}{dx}$ = partial pressure gradient in the x direction	This relationship is Fick's first law expressed in terms of partial pressures of the diffusing component, since gas partial pressures are directly proportional to gaseous molar concentrations. Operational procedures will affect the stagnant boundary layer thickness and density near surfaces, which will affect the diffusion velocities and the concentration gradient.
Molar flux of component A at isothermal conditions, in the direction of flow	OUTPUT: J_A = diffusion flux INPUT: D_{AB} = diffusion of A into a mixture of A and B at a given temperature; R = gas constant; p_A = partial pressure of component A; T = absolute temperature; $\frac{dp_A}{dx}$ = partial pressure gradient in the x direction	This relationship describes molar flux at a constant temperature in the direction of flow, as derived from Fick's first law. Operational procedures will affect the stagnant boundary layer thickness and density near surfaces, which will affect the diffusion velocities, and the concentration gradient.

Equations Describing Selected Individual Phenomena Encountered in Deposits

MECHANISM	INPUT AND OUTPUT PARAMETERS	DESCRIPTION
Molar flux in non-stagnant systems	OUTPUT: N_A =total molar flux of A INPUT: J_A =molar flux due to diffusion through a stagnant layer; c_A =molar concentration of A; V =velocity of bulk past a reference point ($c_A V$ =molar flux past a reference point due to bulk flow)	This relationship describes diffusion in a non-stagnant system, when the bulk is in motion past a reference point. The velocity of A past the reference point is greater than the bulk flow velocity due to the addition of the diffusion velocity (assuming the diffusion is in the direction of flow). Operational procedures will influence the velocity and concentration of the molar flux due to the bulk motion, and temperature and pressure will influence diffusion in the stagnant boundary layer.
Chen and Othmer prediction of diffusion mixtures coefficients for two component gas	OUTPUT: D =diffusivity of the mixture (cm^2/sec) INPUT: T =absolute temperature (K), and T_{cA} and T_{cB} =the critical temperatures of gas A and B, respectively; M_A and M_B = molecular weights of A and B, respectively; p =pressure (atm); V_{cA} and V_{cB} = the critical molar volumes of A and B, respectively ($\text{cm}^3/\text{g-mol}$)	Diffusion coefficients for two component gas mixtures are predicted using the semi-empirical correlation developed by Chen and Othmer (1962). Operational procedures will influence the temperature and pressure of the system.
Eddy diffusivity in turbulent flow	OUTPUT: J_A =molar flux INPUT: E_d =eddy diffusivity; $\frac{dc_A}{dx}$ =molar concentration gradient	Mixing and diffusion occur within the flow stream by the way of eddies as they break up in fragments that then form new eddies. Mixing and diffusion within an eddy may be insignificant when compare to bulk transport and mixing. This expression incorporates transport due to classical diffusion transport and diffusion due to eddy mixing. Operational procedures will influence the eddy diffusive coefficient by way of mass transport parameters (momentum, etc.) and the concentration gradients present.
Facilitated Diffusion in an external force field for small particles	OUTPUT: $\frac{\partial A}{\partial t}$ change of particle concentration A in time INPUT: t =time; v =fluid velocity; D =particle diffusion coefficient; k = Boltzmann const.; T =abs. temp.; $K = \nabla \phi$ =external force acting on particles; ϕ =potential energy of interaction (for example: sum of double layer repulsion energy and London dispersion energy of attraction)	Facilitated diffusion refers to diffusion through a stagnant liquid or gas layer (boundary layer), but it includes intermolecular effects due to double layer repulsion, London dispersion energies of attraction, electrostatic, or magnetic effects. Control of operational and design characteristics can influence fluid velocities, fluid temperature, bulk concentration of A, parameters which influence double-layer formation.

Equations Describing Selected Individual Phenomena Encountered in Deposits

MECHANISM	INPUT AND OUTPUT PARAMETERS	DESCRIPTION
Linear diffusion to a flat surface (Fick's second law)	OUTPUT: $\frac{\partial A}{\partial t}$ change of concentration of constituent A in time INPUT: D=diffusion coefficient and X=distance	This relationship describes linear diffusion to a flat surface through a stagnant liquid or gas layer (boundary layer) without facilitating force fields. This equation assumes the consumption of constituent A at the surface to maintain a gradient. Operational control can influence the concentration of A in the bulk fluid and, indirectly, the boundary layer thickness (x) through which the constituent must move, by changing the bulk fluid velocity.
Fick's second law expressed as a vector function with no chemical reaction between A and B.	OUTPUT: $\frac{\partial A}{\partial t}$ =change in concentration of A with time INPUT: D_A=diffusion coefficient and $\frac{\partial^2 A}{\partial x^2}$ = rate of change of concentration gradient with distance	This equation is a three dimensional diffusion-mass balance with no chemical reaction between A and B, expressed as a vector function. Operational procedures will influence the concentration gradients. In addition, reaction rates and diffusion coefficients are highly temperature and pressure dependent.

Equations Describing Selected Individual Phenomena Encountered in Deposits

MECHANISM	INPUT AND OUTPUT PARAMETERS	DESCRIPTION
Dimensionless Navier-Stokes equation for the Boussinesq approximation Assumptions (energy conservation equation for an incompressible fluid)	OUTPUT: $\nabla' T'$ =dimensionless temperature field gradient INPUT: $\nabla' p'$ =dimensionless pressure field gradient term due to flow – obtained from solving the momentum equation; g=gravity vector; g_c =gravitational constant; w'=dimensionless mass fraction; u' = dimensionless velocity vector-obtained from solving continuity equation; Re = Reynolds number ($\rho D u / \mu$, where D=diameter of flow channel; u=velocity; μ = kinematic viscosity); Gr_t = composition Grashof number $Gr_t = L^3 \beta_t (T_s - T_\infty) g_c / \nu^2;$ L=reference length; T_s=surface temperature; T_∞=bulk temperature; g_c = gravitational constant; ν-kinematic viscosity; $\beta_t = -(1/\rho_\infty)(\partial\rho/\partial T)_{p^\infty, w^\infty}$ $Gr_w = L^3 \beta_w (w_s - w_\infty) g_c / \nu^2;$ L=reference length; w_s=mass fraction at the surface; w_∞=mass fraction in the bulk; g_c = gravitational constant; ν-kinematic viscosity; $\beta_w = -(1/\rho_\infty)(\partial\rho/\partial w)_{p^\infty, w^\infty}$	When natural convection coexists with forced convection (i.e., mixed convection), the relative effect of natural to forced convection is indicated by Gr/Re^2, where $Gr=Gr_t$ or Gr_w. For isothermal mass transfer, $Gr_t=0$, while for uniform composition heat transfer, $Gr_w=0$. The adequacy of the Boussinesq approximations has been tested for natural convection from a vertical plate and for mixed convection from a horizontal plate. The approximations give an adequate representation of velocity and temperature profiles, except near the point where buoyancy causes flow separation. Fluid properties are best evaluated at the reference conditions, although the film condition is adequate for the calculation of average Nusselt and Sherwood numbers. Operational controls will influence the temperature, pressure, mass fraction, density and velocity. The presence of dissolved constituents as well as the temperature will influence the viscosity.
Mass conservation equation for convective transport in a homogeneous medium	OUTPUT: v is the vector velocity (with components u, v, w) INPUT: ρ =density; t= time	The conservation of mass per unit volume Indicates that the temporal change of mass in a volume element is the same as the balance between inflow and outflow plus the mass sources. Operational parameters will influence the mass flow rate, and additions to the flow stream will increase mass flow. Deposition will decrease the mass flow rate.

Equations Describing Selected Individual Phenomena Encountered in Deposits

MECHANISM	INPUT AND OUTPUT PARAMETERS	DESCRIPTION
Momentum conservation equation for convective transport in a homogeneous medium	OUTPUT: p – pressure distribution INPUT: ρ = density; v is the velocity vector (u,v,w), τ = stress tensor, g = gravitational constant, e = unit vector (001), T = temperature	The conservation of momentum indicates that the rate of momentum accumulation is equal to the rate of momentum into and out of the volume element plus the pressure, viscous and gravitational forces acting on the system.
Energy conservation equation for convective transport in a homogeneous medium	OUTPUT: $\nabla \cdot \vec{q}$ = the divergence of the heat flux vector [] tensor products INPUT: ρ = density; $\vec{v}$ = velocity vector = (u,v,w); p = pressure; τ = stress tensor; g = gravitational constant; e = unit vector (0,0,1); $\vec{q}$ = heat flux; u = internal energy unit per mass; ∇ = Laplace operator	The rate of gain of internal and kinetic energy is in equilibrium with the convective rate of energy and the rate of energy transfer by conduction, pressure, viscous and gravitational forces. Operational controls will influence the pressure, density, velocity, heat flux, and the internal energy per unit mass.
Ratio of momentum and heat transfer (Prandtl number)	OUTPUT: $Pr = \frac{c_p \mu}{k}$ INPUT: c_p = specific heat; k = thermal conductivity; μ = absolute viscosity	This equation defines a dimensionless ratio of the momentum to the heat transfer for a flowing fluid. Operational controls will influence the viscosity through the temperature and pressure, and the specific heat and thermal conductivity through control of the constituents present.
Reynolds number	OUTPUT: $Re = \frac{D \bar{v} \rho}{\mu}$ INPUT: D = tube diameter; v = velocity; ρ = density; μ = absolute viscosity	This relationship is a dimensionless ratio that indicates the flow regime of the fluid. Flow below $Re=2,100$ is laminar and can remain laminar up to Reynolds numbers of several thousand, under special conditions of a well-rounded tube entrance and quiescent inflow fluid. Under normal flow conditions, the flow is turbulent at Reynolds numbers above about 4,000. For Reynolds numbers between 2,100 and 4,000, a transition region is found, where the type of flow may be either laminar or turbulent, depending upon conditions at the entrance of the tube and on the distance from the entrance.
Ratio of buoyancy force to change of momentum flux (Rayleigh number)	OUTPUT: $Ra = \frac{g \beta \Delta T I^3}{\nu a}$ $a = k / \rho_0 c_p$; c_p = specific heat; g = gravitational constant; k = thermal conductivity; I = distance; ΔT = temperature differential; β = coefficient of thermal expansion; ρ_0 = density; $\nu = \mu / \rho_0$ = kinematic viscosity; μ = absolute viscosity	This equation describes a dimensionless ratio of the buoyancy force to the change of momentum flux.

B.4 Adsorption and Desorption

MECHANISM	INPUT AND OUTPUT PARAMETERS	DESCRIPTION
Diffuse layer charge	OUTPUT: σ_d =diffuse layer charge INPUT: C=total ionic concentration; $ z $ =modulus of the valence of the supporting electrolyte; ψ_d =potential in the diffuse layer	Gouy-Chapman theory: The developed charge in the diffuse layer is a result of adsorption of potential determining ions and specifically adsorbed anions. Operational control influences the total ionic concentration (and therefore the valance of the supporting electrolyte).
Equilibrium electrical neutrality conditions	INPUT: σ_s =surface charge; σ_i =adsorbed species charge; σ_d =diffuse layer charge	Equilibrium of electrochemical species in the double layer requires charge equilibration to sum zero. Operational controls will influence the ionic concentrations, temperature, pressure, and materials present. Kinetic parameters and fluctuations of system operation will influence the extent of equilibration.
Potential change from the surface to the diffuse layer	OUTPUT: difference between the surface and diffuse layer potentials INPUT: $G = \epsilon_d / 4\pi d$ =is the electrical capacitance of the inner and outer Helmholtz layers; ϵ_d = permittivity of the region; d=thickness of the double layer	The change in potential from the surface to the diffuse layer is the potential change through the double layer. At equilibrium, electrical neutrality will occur, and $\sigma_s + \sigma_i + \sigma_d = 0$. Operational control can influence the temperatures, bulk concentrations and, therefore, ionic strength and temperature at the surface of metals, all of which influence the double layer thickness and overall surface charge.
Stability coefficient equation	OUTPUT: W=stability coefficient INPUT: k_{rapid} =rate constant for the rapid coagulation reaction (no repulsive potential barrier); k_{slow} =rate constant for the slow coagulation reaction	Theoretical evaluation of the rate constant for coagulation requires information on the total interaction energy for particles of a given shape. The rate constants are then converted to the stability coefficient, W. Operational controls will influence the rates of coagulation, as described below for the Fuchs expression.
Kinetic reaction equation for reaction of monomers to dimers, trimers, etc.	OUTPUT: dn/dt = rate of single particle disappearance INPUT: N=number of single particles concentration; D= diffusion coefficient; r_c =critical collision diameter	This relationship is a kinetic equation for the reaction of single particles into dimers, trimers, etc. The rapid coagulation constant is evaluated as if the reaction is a bimolecular, second-order reaction, with no barrier to particle approach, contact, or adherence (i.e., no activation energy to overcome). The rate of coagulation will be controlled entirely by diffusion kinetics and may be described by Fick's Law. Operational parameters will influence the diffusion coefficient (through temperature, pressure, species concentration, etc.) and the number concentration of particles introduced and produced.

Equations Describing Selected Individual Phenomena Encountered in Deposits

MECHANISM	INPUT AND OUTPUT PARAMETERS	DESCRIPTION
Kinetic description of the slow coagulation process	OUTPUT: dn/dt= rate of single particle disappearance INPUT: $V_{\max}$ =height of the activation energy barrier opposing coagulation; n=number concentration of particles; k=Boltzmann constant; T=absolute temperature; r_c =critical collision diameter; D=diffusion coefficient	A slow coagulation process occurs if there is some energy barrier to particle contact and adherence, i.e., if some of the collisions are not “sticky.” The collision process under these conditions can be seen as analogous to a bimolecular reaction in which there is an activation energy to overcome. Operation controls will influence the diffusion coefficient (through temperature, pressure, species concentration, etc.) and the number concentration of particles introduced and produced.
Hamaker constant relating to free energy	OUTPUT: Free energy attraction INPUT: Hamaker constant and distance between particles	The Hamaker constant is a term which is intrinsic to an interacting system that accounts for attractive and repulsive forces between bulk phases and the interference of the intervening medium. The Hamaker constant relates the overall change in free energy of attraction to the separation distance, accounting for the materials and medium. The operational parameters which affect the Hamaker constant include concentration and constituents of the colloidal material, as well as the physical state of the medium (steam).
Hamaker constant relating to ionization potential Effective Hamaker constant in a non-vacuum	OUTPUT: A_H =Hamaker constant INPUT: h=Planck’s constant; α_0=electronic polarizability; v=first ionization potential; n=number of atoms or molecules in unit volume of the phase; v=first ionization potential of the atom or molecules	The value of A_H is related to the energy of the characteristic first ionization potential and the electronic polarizability of the material. This relationship describes surface interactions between similar materials in a vacuum. In most cases, the relevant equations must account for the presence of an intervening medium. Surfaces interrelating through an intervening fluid medium will experience a reduced mutual attraction, due to the presence of the units of the third component. For most purposes, a simple approximation of a composite Hamaker constant is sufficient. When two interfaces of component 1 are separated by a medium of component 2, the effective Hamaker constant (A_H^{eff}) can be approximated by the individual Hamaker constants of the components measured in a vacuum.
Hogg-Healy-Fuerstenau equation double-layer interaction energy	OUTPUT: V_{DL}^{SP} =HHF spherical case solution of the double layer interaction energy INPUT: ϵ =dielectric constant; a=radii of particles; Ψ =potential at separation H_0. k=inverse Debye length	The double layer interaction energy describes the repulsive energy separating the two similar particles. This equation applies for $k\alpha > 10$ for low potentials (<25mV) at large separations. It is assumed that $\Psi_1 \geq \Psi_2 > 0$ or $\Psi_2 \leq \Psi_1 < 0$ (good experimental agreements are obtained when $\Psi_2 \gg \Psi_1$, even though $\Psi_2 \gg 60mV$). Operating conditions will influence the particle radii, particle compositions (and therefore the dielectric constant), particle concentration (and therefore the separation), ionic concentration and constituents (affects the surface charge).

Equations Describing Selected Individual Phenomena Encountered in Deposits

MECHANISM	INPUT AND OUTPUT PARAMETERS	DESCRIPTION
Van der Waals interaction Energy	OUTPUT: V_A^{SP} =spherical case solution of the van der Waals interaction energy INPUT: a=radii of particles; H_0 =distance between surface particles	The van der Waals interaction energy is dependent on the particle separation, radii of the particles and the Hamaker constant for the material. Operational controls will influence the particle radii, particle composition, particle and ionic concentrations and constituents [Hamaker constant being dependent on the particle composition (polarizability of dispersed phase), but independent of the ionic composition of the solution].
Stern Potential from experimentally determined zeta potentials	OUTPUT: Ψ_s =Stern potential INPUT: l=distance of the slipping plane from the particle surface; k_B =Boltzmann constant; T=temperature; e_0 =electronic charge; k=inverse Debye length	In order to calculate the electrical double layer repulsion, proper values for the surface potentials are required. Since electrical double layer interaction arises from the overlapping of diffuse double layers, the surface potentials can be represented by the potential at the boundary between the Stern and diffuse layers. The Stern potential is an essential determination for the computation of the interaction energies, but it cannot be determined directly. The electrokinetic potential (ζ -potential) is commonly used to estimate the Stern potential. The Stern potential is calculated from experimentally determined ζ -potentials by way of the Gouy-Chapman relationship. In this equation, l is on the order of the diameter of the ion adsorbed at the surface (a few angstroms); therefore, the ζ -potential is often substituted for the Stern-potential, although the two need not be the same. The ζ -potential can never be higher than the Stern potential, and therefore, as seen from the equation, when $\Psi_s = \zeta$, the theoretical stability coefficient calculated is always the lowest value possible. The operational parameters which will affect the Stern potential (and ζ -potential) are the electrolyte concentration, temperature, colloid and surface materials, and colloid concentration (average separation distance).
Kinetics of chemisorption at interfaces	OUTPUT: dq/dt adsorbate taken up in time, t INPUT: a = const. relating to the initial velocity of reaction; b=const. relating to activation energy for adsorption	The Elovich equation describes the kinetics of chemisorption at interfaces. Operational control influences bulk concentrations of adsorbate and, therefore, indirectly affects the initial velocity of the adsorption reaction.

Equations Describing Selected Individual Phenomena Encountered in Deposits

MECHANISM	INPUT AND OUTPUT PARAMETERS	DESCRIPTION
Rate of decrease of adhered particles	OUTPUT: $\frac{dN_d^s}{dt}$ - Where N_d^s =number of detachable adhered particles and t=time period INPUT: p=rate constants of detachment and relocation (subscripts d and b, respectively); N=number of release particles;; N_b^s =number of relocated particles	In systems with substrates of rough surfaces, surface relocation of particles must be considered. The rate with which the number of detachable adhered particles, dN_d^s / dt , decreases is equal to the sum of the rates of escape into the solution bulk and of relocation of particles on the surface into a permanently bound state. Operational controls will influence the number of particles present; the rates of attachment, detachment, and relocation through the water (or steam) chemistry; flow rates; temperature; and surface characteristics.
Apparent rate constant	OUTPUT: k' =apparent rate constant INPUT: p_d =rate of detachment; p_b =rate of relocation	This relationship defines the apparent rate constant of particle removal from a surface. The absolute values of p_d and p_b cannot be ascertained; however, a relative p_d can be determined by $p_{d,rel} = x_\infty k'$ (x_∞ =fraction of released particles at infinite time). Operational controls will influence the rates of attachment, as described for the rate of decrease of adsorbed particles.
Total interaction energy per unit area (E_{tot}) in the absence of external fields	OUTPUT: E_{tot} =total interaction energy INPUT: E_B =Born repulsion energy; E_{vdW} =van der Waals attraction energy, E_{el} =electrostatic energy	The interaction energy of particle detachment from surfaces is short range in nature, resulting in the necessity to consider the Born wall repulsion together with the more common electrostatic and van der Waals energies. The interaction energy E_{tot} is essentially obtained from two potentials: molecular and electrostatic. The former is taken as the classical Lenard-Jones 6-1 2 potential, which gives both the van der Waals and Born repulsion terms in E_{tot} . The ranges and the relative magnitude of various components of E_{tot} differ considerably. At very short separations, the dominant term is E_B . It represents a very powerful repulsion, the effect of which is only felt when the particles almost touch each other; it is hardly felt beyond 20 Å. The van der Waals attraction is a long range effect, and its influence is felt over all separations of interest. The electrostatic interaction energy is complex, depending on the ionic strength, pH, and separation distance. Operational controls will influence the interaction energies through the particle size, particle concentration, materials present, temperature, pH, and ionic strength and consistency.

B.5 Thermodynamic Equations for Surfaces – Chemistry Exchange Across Phases and Concentration in Droplets

MECHANISM	INPUT AND OUTPUT PARAMETERS	DESCRIPTION
Kelvin equation Kelvin equation for components over a curved surface	OUTPUT: μ_i =chemical potential INPUT: P=pressure; R=gas constant; T=temperature;; μ_i^0 =chemical potential at standard conditions; $\ln\left(\frac{P_i}{P_i^0}\right) = \frac{2v_i\gamma}{rRT}$ P_i =vapor pressure of the ith component over a planar surface; P_i^0 =vapor pressure of the ith component over a curved surface; v_i =partial molal volume of the ith component; γ =surface tension; r= radius of droplet	These equations describe the chemical potential for a vapor above the planar surface of a liquid. This equation applies to the chemical potential related to vapor pressure over a curved surface of radius r. As the radius of the droplet decreases, the vapor pressure above it increases, i.e. the concentration of the material in the gas phase is higher near the surface of the droplet, and, therefore, the concentration of the material in the droplet is higher, keeping it in the droplet longer. Operational parameters will influence the components present, temperature, and the pressure of the system.
LaPlace equation	OUTPUT: $(P_g - P_l)$ INPUT : γ =surface tension; r = radius	The LaPlace equation for a bubble of gas in a liquid defines the difference between gas and liquid pressure, AP, across the interphase. Operational parameters will influence the pressure and temperature (surface tension).
Variation of surface tension with temperature	OUTPUT: γ =surface tension INPUT: T=absolute temperature; T_c =critical temperature;; γ_0 =surface tension at 0 K	This is an empirical equation to predict the variation of surface tension with temperature for non-polar liquids.

Equations Describing Selected Individual Phenomena Encountered in Deposits

Work of adhesion between two phases	OUTPUT: W^{123} =work of adhesion between two liquid phases and a third vapor phase INPUT: γ^{13} =surface tension for first liquid in contact with a vapor; γ^{23} =surface tension of second liquid in contact with a vapor; γ^{12} = surface tension between the two liquids	The work of adhesion between two phases is defined as the work necessary to separate unit areas of those surfaces. Operational parameters will influence the interfacial surface tension, through temperatures, pressures, and constituents present.
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B.6 Kinetics of Deposition

MECHANISM	INPUT AND OUTPUT PARAMETERS	DESCRIPTION
Dimensionless deposition rate of particles or ions	OUTPUT: η_R =dimensionless deposition (or removal rate) INPUT: α =attachment (or detachment) efficiency; η_T =dimensionless transport rate	The attachment efficiency (α) accounts for chemical-colloidal effects on the rate of deposition, while η_T accounts for physical effects. When chemical-colloidal interactions are favorable for deposition (i.e., in the absence of repulsive total interaction energies), the attachment efficiency approaches unity, and the deposition rate is equal to the transport rate. In this case, particle transport is the rate-determining step; this case is generally referred to as favorable deposition. Operational controls influence the rate of transport to the surface and the rate of attachment through temperature, materials, and solute/colloid concentrations.
Chemical-colloidal effects on the attachment efficiency	OUTPUT: α_{the} =attachment efficiency [proportional to $\exp(-\phi/kT)$, k=Boltzmann constant; T=abs. temp.; ϕ =total interaction energy as determined by the chemical characteristics of solid-solution interfaces] INPUT: C_S =electrolyte conc.; B=numerically evaluated function that depends on the surface potential of particles and collectors(ψ_p, and ψ_c, respectively); z= valence of the counterions; a_p =radius of suspended colloids	This relationship is a theoretical prediction of the effects of solution chemistry and colloidal interactions on the attachment efficiency. In this equation, the slope of $\log \alpha_{the} - \log C_S$ curves is dependent on ψ_p, ψ_c, z, and a_p. This theory predicts a linear dependence of the slope of $\log \alpha_{the} - \log C_S$ curves on a particle size (radius). Operational controls influence the electrolyte concentration and surface chemistry (materials).

Equations Describing Selected Individual Phenomena Encountered in Deposits

MECHANISM	INPUT AND OUTPUT PARAMETERS	DESCRIPTION
Monolayer deposition at breakthrough coordinates	OUTPUT: $C_{(X,\tau)}$ =colloidal concentration for monolayer deposition at breakthrough coordinates (X, τ) INPUT: C_0 =inlet concentration; f=ration of total surface area to void volume; K_m =mass transfer coefficient; $x=z/v$. where z=position in reactor and v=average flow velocity; α =monolayer adhesion efficiency parameter; $\tau = t - z / v$, where t=time; a=average area per particle	Parameters α and a can be obtained experimentally. α was defined phenomenologically as the ratio of the actual mass transfer coefficient to the ideal convective-diffusion value. A possible discrepancy for applying this model in the case of deposition over a high energy barrier is that detachment effects may not always be negligible. Detachment is usually negligible in the rapid deposition range (RDR), where RDR is the regime when the energy barrier is decreased by increasing ionic strength, or if the adhesion is enhanced by long-range forces (e.g. magnetic). α in the RDR is in the range 0.3-0.7. Operational controls influence the inlet concentration of material, diffusion coefficient (through temperature, pressure, flow rate and other parameters that influence the boundary layer thickness), materials and surface area of the system.
Collector surface/particle area ratio	OUTPUT: Y=area ratio INPUT: $\Gamma_{\max}^{(1)}$ =saturation surface concentration of adhered particles in the first layer; r_{particle} =radius of the particles; π =pi; θ =covered surface relative to the surface area	Particle-particle interactions which may prevent close approach of particles in a monolayer have a ratio of y. In monolayer adhesion $y \approx 1.10$. Operational controls influence the particle size and surface area of the system.
Fraction of bare surface	OUTPUT: F_0 =fraction of bare surface INPUT: a=average area per particle, $1/\Gamma_{\max}$ ($\Gamma_{\max}$ =maximum particle monolayer coverage)	This relationship describes the fraction of the surface not covered by adsorbed monolayer. Operational controls influence the factors which influence $\Gamma_{\max}$ (ionic strength, temperature, materials, concentration, particle particle interaction, and long range forces.
Surface flux of particles for monolayer coverage	OUTPUT: surface flux of particles $\frac{\partial \Gamma}{\partial t}$ INPUT: a=surface area ratio; C=particle concentration; K=diffusion coefficient; t=time; α =monolayer adhesion efficiency parameter; Γ =particle coverage (particles per unit area of surface)	This equation assumes that no detachment of material once it is at the surface and that the adhesion of particles does not affect (deplete) the bulk particulate concentration. Operational controls will influence the diffusion coefficient, the bulk concentration of particulates, the surface area ratio, and the factors which influence the adhesion efficiency and particulate coverage (ionic concentration, pH, temperature, materials, etc.).

B.7 Potential of Zero Charge (PZC)

MECHANISM	INPUT AND OUTPUT PARAMETERS	DESCRIPTION
Surface charge on metal per unit area	OUTPUT: Surface charge q^m INPUT: F = Faraday constant; z_i = is the charge of the ionic species, i (including the sign); and Γ_i is the surface excess of that component in the interphase, in moles per unit area of the interface. The summation is limited to the solutions side of the double layer	A metal immersed in a solution of an electrolyte facilitates the formation of a double layer at the interface, such that there can be an excess charge on the metal side of the interface and an ionic atmosphere with a net excess of one kind of ions in the solution side of the double layer, to maintain electro neutrality over all of the system. The charge on the solution side of the double layer q^s is the equal and opposite in sign to the charge on the metal ($q^m = q^s$). Operational controls influence the materials used, electrolyte concentration, and temperature of the surface and solution.
Dependence of the free energy of adsorption of a dipolar solvent on the field F in the double layer	OUTPUT: F = Field in the double layer INPUT: q^m = charge density on the metal; $\mathcal{E}$ = dielectric constant	Electrosorption can be viewed as a replacement reaction (i.e. competition between solvent and solute for surface sites), and it is dependence of the free energy of adsorption of the dipolar solvent on the field, F, in the double layer. Operational control influences the materials used, electrolytes presence (and therefore the double layer thickness), and the temperature.
Physicochemical properties of the metal	OUTPUT: $E_{q=0}$ = potential of zero charge INPUT: D = density of the metal; A = atomic weight; n = no. of free electrons in the metal per nucleus	This equation uses empirical relationships for the bulk properties of a metal and its surface properties to predict its potential of zero charge. The quantity on the left hand side of the equation is the free electron density in the metal. It should decrease with increasing temperature, due to the decrease in density. This equation is claimed to be useful in the range of $E_{q=0} = 0.6$ to -1.1 V (NHE). Operational control influences include the temperature and the materials used.

B.8 Multilayer Deposition

MECHANISM	INPUT AND OUTPUT PARAMETERS	DESCRIPTION
Particle number conservation	OUTPUT: C=average particle number concentration per unit volume INPUT: f= ratio of the total surface area in the column to the void volume; t=time; v=average flow velocity in the column; z=position down the collection column; Γ=average number of particles deposited on the collector surface	This equation describes multilayer deposition considered in a vertical column of height Z ($0 \leq z \leq Z$). Deposition is considered only under the influence of convective diffusion. Operational controls will influence the concentration of particles, velocity of the particles, and the geometry of the system.
Average area per particle in the first layer	OUTPUT: a - average area per particle in first layer INPUT: $\Gamma_{\max}^{(1)}$=maximum particles coverage per unit collector surface area	In the case of monolayer adsorption, $\Gamma_{\max}^{(1)}$ is the saturation value of Γ . a is the average area per particle in the first layer. Operational controls will influence the particle concentration, system geometry, and the chemical and surface conditions that influence colloid adsorption.

Equations Describing Selected Individual Phenomena Encountered in Deposits

MECHANISM	INPUT AND OUTPUT PARAMETERS	DESCRIPTION
Adhesion efficiency parameters	OUTPUT: $flux$ - rate of particle adherence per unit area INPUT: α = adhesion efficiency parameter for particles reaching bare collector surface; $C(z,t)$=particle concentration at position z at time t; $flux$=number of particles that adhere at the collector surface per unit time and per unit area; K_m=mass transfer coefficient(ideal case convective-diffusion deposition only) If based on the fraction of the bare surface, F_0, adhered in layer 1 on the bare collector surface: OUTPUT: $flux$ - rate of particle adherence per unit area INPUT: α =adhesion efficiency parameter; F_0 =fraction of bare surface; K_m =mass transfer coefficient; C=concentration of particles For layers adhered in layers $(n+1)$ on top of $n>0$ layers, the flux is as follows: OUTPUT: $flux$ - rate of particle adherence per unit area INPUT: β =adhesion efficiency for particles reaching the parts of the surface already covered by other particles; $F_{n>0}$ =fraction of surface covered by n layers ($n>0$)	The flux is based on the assumption that no detachment occurs (i.e., attachment is irreversible). The adhesion efficiencies for the multilayer adsorption may be modified to reflect particle detachment by varying the adhesion probabilities for differently n-layers (β varies with n-layers). The rate equations for adhesion to the different layers are obtained by differentiating the fraction of surface coverage for the n layers with respect to time. Operational controls will influence the particle concentration and factors affecting the convective diffusion (temperature, velocity, density, concentration gradient, surface area, etc.).

Equations Describing Selected Individual Phenomena Encountered in Deposits

MECHANISM	INPUT AND OUTPUT PARAMETERS	DESCRIPTION
Combined rate equation for multilayer adsorption	OUTPUT: Rate of Particle Adhesion $\frac{\partial \Gamma}{\partial t}$ Where Γ =particle coverage (number of particles per unit collector surface area) INPUT: C=particle concentration; F_0 =fraction of the bare surface; K_m =mass transfer coefficient; t=time; α =adhesion efficiency parameter; β =adhesion efficiency for particles reaching the parts of the surface already covered by other particles	This equation describes the rate of particle adhesion to collector surface per unit area for both the initial and subsequent layers for the model, which assumes a constant adhesion efficiency (initial layer, α, and subsequent layers, β). Operational controls influence the particle concentration, mass transfer (temperature, pressure,(density, viscosity), velocity, boundary layer thickness, etc.),surface area, and chemical and ionic conditions, which will affect the adhesion efficiencies.
Surface coverage	OUTPUT: Γ =surface coverage (particles per unit collector surface area) INPUT: a=surface area ratio; F_0 =fraction of bare surface; α =monolayer adhesion efficiency parameter; β =multilayer adhesion efficiency parameter	The equation defines surface coverage Γ in terms of the fraction of bare surface and efficiency parameters. If the suspension is stable, i.e. the particle-particle interactions involve a repulsive barrier, $\beta \ll 1$. At the critical coagulation conditions (CCC), $\beta = 1$. The use of a single parameter, β, to describe multilayer adhesion implies neglect of the possibility of different types of adhesion sites, depending on the local morphology of the already existing particle layers on the surface. In this concern, this model is similar to the BET theory of adsorption. Operational controls will influence the parameters that affect adhesion efficiency, surface area, and surface coverage (ionic strength, pH, temperature, etc.).

B.9 Particle Electric Field Interaction and Particle Settling

MECHANISM	INPUT AND OUTPUT PARAMETERS	DESCRIPTION
Stokes law	OUTPUT: $\frac{dv_p}{dt}$ - change in acceleration of a particle INPUT: m_p =particle mass; v_p =particle velocity; a=initial particle acceleration; μ_g =medium viscosity; d_p =particle diameter	When the velocity of the medium is much less than the acoustic velocity, then the values of all the forces represented by F_{MA} are negligible compared with other forces. If the density of the medium is not significant compared to the particle density and the particle velocity is much greater than the gas velocity (which occurs for particles which deposit), then Stokes law can be applied. The momentum conservation, Stokes law, states that the change in acceleration results from subtracting from the initial particle acceleration the change due to buoyancy. Operational influences include fluid velocity, temperature and pressure (influencing acoustic velocity), particle materials and characteristics, particle acceleration forces, and gas viscosity.
Relaxation time	OUTPUT: τ =relaxation time INPUT: v_p =particle velocity; a=particle acceleration relative to the medium	The relaxation time is the interval under which most of the change in particle motion takes place. The initial steady-state is either an at-rest or in-motion condition. At the point where time $t = \tau$, a particle being accelerated reaches approximately two-thirds the terminal velocity, and a particle being decelerated reaches about one-third the initial velocity. Operational parameters influencing the relaxation time include the mass velocity of the bulk stream (particle velocity), the forces acting on the particle (magnetic, electrostatic), and temperature and pressure of the bulk fluid (resistance to a change in flow).
Terminal settling velocity of a particle	OUTPUT: v_s =particle terminal settling velocity INPUT: v_p =particle velocity; t=time; τ =relaxation time; a=acceleration	The solution to the first order differential equation for any Stokes particle moving due to an external force with acceleration starting from rest (relative to the medium) describes the terminal settling velocity. Operational influences include bulk fluid velocity and strength of influencing forces.

B.10 Solutions of Gases in Liquids

MECHANISM	INPUT AND OUTPUT PARAMETERS	DESCRIPTION
Temperature effect on gas solubility	OUTPUT: c=concentration of moles of dissolved gas in liters of solution INPUT: T=temperature; ΔH= differential heat of solution (enthalpy of solution); R=gas constant	The solubility of a gas in a liquid is dependent on the temperature and pressure of the system and the nature of the gas and liquid. An increase in pressure increases the mass of gas dissolved, whereas an increase in temperature decreases the mass of dissolved gas in solution. The process of dissolving a gas in water generally involves the liberation of heat. For an ideal gas at constant pressure, the equation presented describes the thermodynamic relationship. Operational controls will influence the temperature and pressure of the system and the concentration of gas present dissolved in the water phase.
Change in dissolved gas concentration with temperature	OUTPUT: $\ln \frac{c_2}{c_1}$ Where c_1, c_2=concentration of dissolved gas in solution at temperatures T_1 and T_2, respectively INPUT: R=gas constant; ΔH= differential heat of solution (enthalpy of solution)	If ΔH is considered to be independent of temperature, the integration of the prior equation between temperatures T_1 and T_2 results in the presented relationship. Although it is generally true that an increase in temperature is accompanied by a decrease in solubility of a gas, some soluble gases (i.e. hydrogen and inert atmospheric gases) may not follow this general relationship, especially in nonaqueous solvents. Operational controls will influence the temperature and molar concentration of the dissolved gases through concentrations present and pressure of the system.
Henry's Law pressure effects on gas solubility in solution	OUTPUT: m=mass of gas dissolved by a unit volume of solvent INPUT: k=constant; p=equilibrium pressure	Henry's law states that the mass of gas dissolved by a given volume of solvent, at constant temperature, is proportional to the pressure of the gas with which it is in equilibrium. Operational controls will influence the temperature, pressure, and constituents present.
Distribution ratio	OUTPUT: <u>concentration of gas:liquid phase</u> concentration of gas:gaseous state =constant	According to Henry's law, m/p is constant; therefore, at a given temperature, independent of pressure, the ratio of the concentration of gas in the liquid phase to the concentration of gas in the gaseous phase is constant. The constant is described as the distribution ratio. The solubility of gases in liquids obeys satisfactorily this relation for gases of low solubility, provided the pressures are not too high or the temperatures too low. These generalizations are strictly applicable to ideal systems, and any departure from ideal behavior will result in deviations from Henry's law. Deviations from Henry's law are also to be expected when differences between molecular complexity are encountered in the gas and liquid phases by compound formation between solute and solvent and ionization processes. Operational controls will influence the temperature and pressure of system. The constituents present will each contribute to the vapor and liquid phases and deviate from ideallity in some intrinsic way.

B.11 Non-Ideal Behavior of a Component in Solutions

MECHANISM	INPUT AND OUTPUT PARAMETERS	DESCRIPTION
Chemical potential	OUTPUT: μ - chemical potential INPUT: p=partial pressure(fugacity of nonideal gas) of the component in the vapor in equilibrium with the solution; R=gas constant; T=temperature; x=mole fraction of component in solution; μ^0, μ_x^0 = chemical potential at standard conditions, and chemical potential of component x at standard conditions, respectively	This equation describes the chemical potential of a component in a solution. For ideal solutions, the partial pressure (fugacity) is proportional to the mole fraction(x) of that constituent of the solution. μ_x^0 for a given substance is constant, at a given temperature and pressure, and is independent of the composition of the solution. Operational controls will influence that temperature, pressure, and in addition, the mole fraction of the solute in the solvent (steam).
Activity coefficient for Raoult's law	$a = xf$ OUTPUT: a=activity coefficient INPUT: x=mole fraction; f=activity coefficient	Non-ideal solutions require a modification of Raoult's Law by the incorporation of an activity coefficient. The activity of a non-ideal solution can be expressed as a product of the activity coefficient and mole fraction (x) of a dissolved species. The chemical potential can then be expressed as a function of the activity coefficient. The reference chemical activity is arbitrarily chosen at a standard state to give an activity of one. The activity of a component in any solution is expressed as a ratio of the activity in the standard state. Therefore, the activity of a solution approaches one (the ideal solution activity), as the solution tends towards infinite dilution. The activity can, therefore, be defined in three alternative ways, the activity becomes equal to: 1) the mole fraction, 2) the concentration, or 3) the molality of the solute as infinite dilution is approached. Operational controls will influence the temperature, pressure, and mole fraction of solute in the steam phase.

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