HEXAVALENT CHROMIUM AIR DISPERSION MODELLING IN THE SOUTH AFRICAN FERROCHROMIUM INDUSTRY

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ABSTRACT

The need to establish and harmonise methodologies to quantify air emissions, atmospheric dispersion and the consequences of air pollutants (especially hexavalent chromium) from the ferrochrome industry became important aspects with the increasing demands for comprehensive impact assessments.

The paper includes a synthesis of current knowledge on the following aspects:

- *Locally and internationally accepted methodologies for the quantification of chromium emissions, including sampling methods and emission factors;*
- *A compilation of recognised and accepted air quality sampling and laboratory analysing techniques; and,*
- *Dispersion modelling and impact assessment tools.*

Depositing and removing materials from the chromium ore stockpile and wind erosion of exposed stockpiles result in mainly chromite emissions unlikely to contain significant amounts of hexavalent chromium. Pre-treatment processes such as drying, crushing and screening also produces chromium emissions, but mainly as trivalent chromium. The smelting of chromium is the major source of chromium emissions - open furnaces have the highest uncontrolled chromium emissions, followed by semi-closed and closed furnaces, respectively. Based on the current knowledge on emission rates, interim emission factors for particulate, total chromium and hexavalent chromium releases are provided.

Ambient sampling and analytical methods to determine environmental exposure of the general public require that hexavalent chromium needs to be quantified in very low concentrations. Suggested sampling and analytical methods for both source characterisation and ambient monitoring are provided.

The selection between dispersion models needs to be based on the size of the modelling domain and the complexity of the terrain. The discussion on dispersion models includes the US EPA's Industrial Source Complex Model (Version 3), the AERMET/AERMOD suite of models and the CALMET/CALPUFF suite of models.

Guidelines are also proposed for environmental exposure assessments including cancer and non-cancer health effects.

1. INTRODUCTION

Chromium as a metallic element was first discovered more than two hundred years ago by Nicolas-Louis Vauquelin, a professor of chemistry and assaying at the School of Mines in Paris. His analysis of some samples of crocoite ore (a lead chromate or $PbCrO_4$) in 1797 revealed a new metallic element, which he called chromium after the Greek word khrôma, meaning colour. After further research he detected trace elements of chromium in precious gems - giving the characteristic red colour of rubies and the distinctive green of emeralds, serpentine, and chrome mica.

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Mining of chromium ore started in Southern Africa around 1906. Recent consumptions figures released by the International Chromium Development Association indicate a split of 85%, 8% and 7% between metallurgical, chemical and refractory industries, respectively. South Africa accounts for 47% of annual world needs whilst Kazakhstan and India provide 18% and 13% respectively.

2. CHROMIUM AIR EMISSIONS

Ferrochromium is produced by the pyrometallurgical reduction of chromite ore with carbon and/or silicon in high temperature electric arc furnaces. A generalised flow chart of the electric arc furnace method of ferrochrome production is shown in Figure 1. The principal smelting process includes the preparation of the chromite ore, the furnace, gas cleaning equipment and the product handling and sorting plant.

Chromite ore and other necessary raw materials are brought to the plant and stored in stockpiles. Depositing and removing materials from the chromium ore stockpile and wind erosion of exposed stockpiles result in emissions of chromite particulates. These emissions are unlikely to contain significant amounts of hexavalent chromium. Storage piles can be sheltered by walls, covered or sprayed with water to reduce emissions.

The ore may need to be dried before being crushed, screened and blended with the other raw materials. Fines or ground ore may also be briquetted or pelletized with bentonite. These may then be roasted (e.g. rotary kiln) or sintered (e.g. steel belt furnace). Pre-treatment processes, such as drying, crushing and screening also produce chromium emissions. Some operators control these emissions using wet scrubbers, cyclones and bag filters.

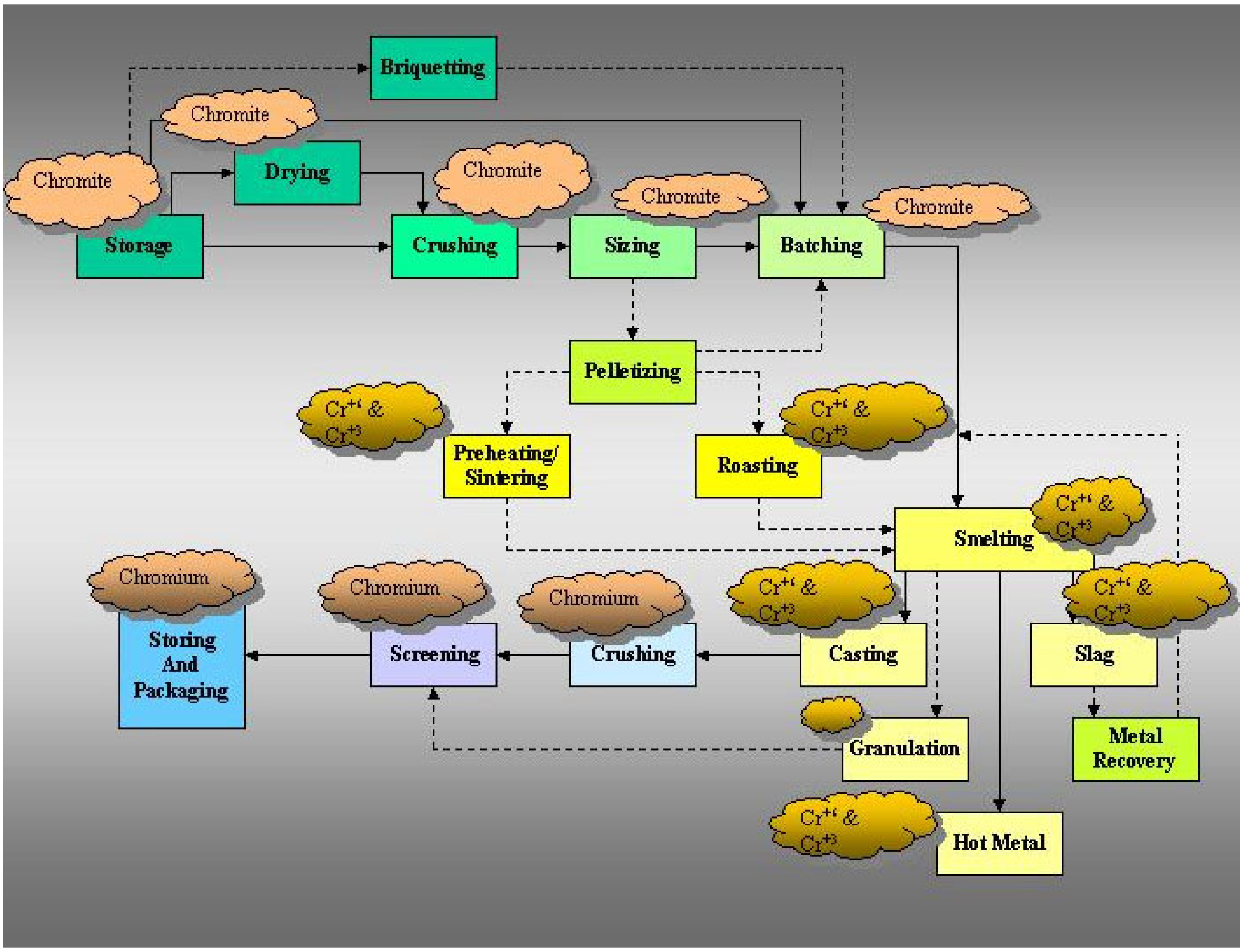

Figure 1. Simplified flowchart indicating potential locations of chromium emissions.

The smelting of chromium in the electric arc furnace is the major source of chromium emissions. Three types of electric arc furnaces may be used. These include open, closed (or sealed) and semi-closed (or semi-sealed) furnaces. Open furnaces are the most common type of electric arc furnaces. The main advantages of this type of furnace include the ability to stoke it during operation and the flexibility to manufacture several types of ferroalloys without altering furnace designs. Open furnaces have the highest uncontrolled chromium emissions because the large opening between the furnace rim and hood allows more circulation of air and gases through the charge material, which entrains chromium and other particulates. A fume collection hood is usually located anywhere from 1.0 m to 2.4 m above the top of the furnace shell. Off-gas from open furnaces is completely combusted on the surface of the furnace burden. Dust and fumes from the smelting process are drawn into the hood along with large volumes of ambient air. These emissions are normally routed to cyclones followed by bag filters. Fumes and particulates may escape if adequate draft is not maintained in the collection hood. The reported efficiencies of removing chromium-containing particulates in bag houses are typically 98% to 99% with availabilities, typically 96% to 99%. Under upset conditions, these gases would be emitted through emergency stacks.

In the closed furnace type, packing is used to seal the cover around the electrodes and charging chutes. The furnace is not stoked and a slight positive pressure is maintained to prevent air getting into the furnace. No combustion of the off-gas takes place, hence reducing the volume of gas requiring collection and treatment. Wet scrubbers (e.g. venturi scrubbers) are used exclusively to control exhaust gases from closed furnaces. These scrubbers capture a substantial percentage of the pollutants. According to Outokumpu, particle removal efficiencies of 99.6% are typical. In their design, two venturi scrubbers are available for each furnace - the design specification is such that a single scrubber could adequately recover all off-gas. Furthermore, the suppliers of the scrubbers offer 96% availability per scrubber. The overall scrubber availability is therefore near 99% due to the duplication of the system.

Due to its high calorific value (as carbon monoxide), the off-gas is reused in various process stages, such as sintering and preheating furnaces. Excess clean gas is flared off. Since the furnace provides a reducing environment, any chromium in the off-gas would be in the trivalent state. However, the combustion of the carbon monoxide-rich gas in the heating and sintering processes, and the burning of the excess gas in the flare could oxidise this chromium to the hexavalent state. Wet scrubbers are often used to clean emissions from the drying and sintering processes. Since hexavalent chromium is highly water soluble, it is reasonable to assume that when this is present in small quantities, no significant emissions would occur. The two locations of significant emission from closed furnaces would therefore be the flare and fugitive emissions during the tapping operation. Estimating emissions from both of theses sources is, unfortunately, not easily done. Outokumpu theoretically estimated the formation of hexavalent chromium in the flare. The total chromium content of the furnace off gases was given as 1 to 5%. According to Outokumpu, less than 1% of this amount will be converted to hexavalent chromium. The fumes from the taphole may be extracted via an overhead hood and ducted to appropriate control devices. It is important that the duct and hood design would have a capture velocity sufficient to remove the fumes. These emissions are intermittent and take place 10% to 15% of the furnace operating time. Current information, however, does not allow an estimate to be made of these emissions.

The cover for closed furnaces has holes for the charge and electrodes to pass through. When these hood openings have mechanical seals around the electrodes and sealing compounds around the outer edges, such furnaces are referred to as “totally closed” or “sealed” furnaces. Closed furnaces that partially close the hood openings with charge materials are referred to as “semi-closed” and “semi-sealed” furnaces. Although these covered furnaces significantly reduce air infiltration, some combustion still occurs under the furnace cover. Off gases and entrained chromium-containing particles are drawn from beneath the cover through ducts leading to the control device. Fugitive emissions may escape through the openings around the electrodes; however, hoods can be placed above the furnace to entrap these emissions. Control devices include wet scrubbers and fabric filters.

Additional emissions occur as the product is finished. After smelting and tapping, the ferrochromium is cast. Chromium-containing particles and fumes escape as the molten product is poured into moulds. Other sources include the final crushing, sizing and packaging.

The USA-EPA provided emission factors for total chromium based on the results obtained at three plants in a 1974 EPA report. The total chromium emission factor for an open furnace producing high-carbon ferrochrome controlled with a fabric filter was given as 0.0022 kg/MWhr, or 10 g/t (assuming 0.21 t ferrochromium production per MWh). The US EPA provided no emission factors for closed ferrochromium furnaces.

Using a combination of both controlled and uncontrolled emission sources, emission factors for finishing operations and product handling were also included in the US EPA recommendations. These are summarised in Table 1. Only 25% of the sources used to determine the emissions from ladle treatment were controlled. Approximately 42% of the casting sources were controlled, while 93% of the sources used to determine the crushing and grinding of product composite factor were controlled. These emission factors are expressed in terms of total elemental chromium, and no split between trivalent and hexavalent oxidation states was given.

Table 1. US EPA emission factors for finishing operations and product handling.

Emission Source	**Total Chromium (g/ton product)**
Treatment of molten alloy with chlorine or other gas in ladle	3 300
Casting of ferrochrome product	70
Crushing/Grinding of product	210

Emissions of chromium from the processing of raw material would predominantly be in the trivalent oxidation state. As for the emissions for finishing operations and product handling, the US EPA developed emission factors of chromium from raw material handling on a combination of both controlled and uncontrolled emission sources. These are summarised in Table 2. Only 15% of the sources used to determine the emissions from storage were controlled, while 75% of the sources included in drying, crushing and sizing were controlled. 20% of the sources included in the weighing and feeding processes were controlled.

Table 2. US EPA emission factors from processing of raw materials.

Emission Source	**Total Chromium (g/ton ore processed)**
Receipt and storage of chromium ore in stockpile	340
Drying, crushing and sizing of chromium ore	340
Weighing and feeding chromium ore to furnace	310

The analysis of stack and baghouse sampling campaigns at a number of South African ferrochrome smelters allowed the calculation of emission factors for particulate matter, chromium (total) and hexavalent chromium. Although there is still much debate around the validity of the sampling results, a summary of these factors, albeit preliminary, is provided in Table 3, below.

The emission factor for the open furnace of 17.4 g/t is slightly higher than the value provided by the US EPA of 10 g/t.

Table 3. Estimated chromium emission factors for electric arc furnaces (g/ton of ferrochrome product).

Furnace Type	**Total Particulates**	**Total Chromium**	**Hexavalent Chromium**
Closed:			
Clean Gas Stack	10 213	496	~0.0
Raw Gas Emergency Stack	16.3	0.8	0.007
Open and Semi-Closed:			
Baghouse	148	17.4	0.06
Emergency stacks	91 000	43	8.1

3. SAMPLING AND ANALYTICAL METHODS

3.1 Ambient Air Sampling

Sampling ambient air to determine community exposure to hexavalent chromium requires fairly high volumes of air, adequate enough to collect a sample that can be detected. A summary of analytical methods is given in Table 4. These methods were generally developed for occupational exposure as seen by their relatively high detection limits. For a cancer risk of one in a hundred thousand, hexavalent chromium has to be quantified in the range of 0.1 to 1 ng/m3. Only a number of the methods are therefore applicable.

Sample recovery includes a post-sampling nitrogen purge of the impinger train as a safeguard against the conversion of hexavalent chromium to another valance state, and filtration of the liquid sample to remove insoluble matter, including the majority of trivalent chromium that is present. When total chromium is determined, the filter residue is retained for analysis. Otherwise, it is discarded.

The impinger train samples are analysed for hexavalent chromium by using an ion chromatograph equipped with a post-column reactor (IC/PCR) and visible wavelength detector. The IC/PCR separates the hexavalent chromium as chromate from the other components in the sample matrices that may interfere with the hexavalent chromium-specific diphenyl-carbazide reaction that occurs in the post-column reactor. To increase sensitivity, a pre-concentration system may be used in conjunction with the IC/PCR.

The method cannot be used as designed for sampling of hot sources, because the alkaline recirculating liquid evaporates in the aspirator, leading to the deposition of salts in the system. In most cases the aspirator part can be left out, without compromising the accuracy of the method. In isokinetic sampling of stacks, the linear velocity of gas through the sampling nozzle and probe is so high that reduction would not occur to an appreciable extent at such low residence times in the train.

3.2 Sampling and Analytical Methods for Source Characterisation

3.2.1 USEPA Method 0012 (Metals)

Commonly known as the multiple metals method, Method 0012 was developed for the determination of multiple trace metals in emissions from hazardous waste incinerators and other combustion sources. The method can also be used for sampling of other point sources. Sampling is conducted using a Method 5 isokinetic sampling train, modified to include a low metals background quartz-fibre filter, a Teflon® frit, glass nozzle and probe, and extra impingers with special absorbing reagents. The gaseous substances and particulates are withdrawn isokinetically from the source. Particulates are collected in the probe and on the filter, and gaseous substances in the chilled impinger set. The sampling train components are recovered in separate front- and back-half fractions, using conventional (including Parr® Bomb) or microwave techniques. Analyses are conducted with various techniques of atomic absorption spectrometry (AA), inductively coupled plasma optical emission spectrometry (ICP-OES), or inductively coupled plasma mass spectrometry (ICP-MS). An important consideration in the use of this method is that it does not allow for speciation of the various metal compounds or valence states. For chromium, therefore, total chromium would be reported.

3.2.2 Method Cr+6

A method known as Method Cr^{+6} has been developed for the determination of hexavalent chromium emissions from hazardous waste incinerators, municipal waste combustors, sewage sludge incinerators, and boilers and industrial furnaces that burn hazardous waste. The method may also be used for the determination of total chromium emissions. Sampling is conducted isokinetically from the emission source. To eliminate the possibility of reduction of hexavalent chromium in the sampling train between the nozzle and the impingers, the emissions are collected with a recirculatory train where the alkaline impinger reagent is continuously circulated through an aspirator to the nozzle. Otherwise the sampling train is based on the Method 5 train, but without a filter. The components of the train are constructed mainly of Teflon® to minimise interaction of the hexavalent chromium with glass. Some glass, quartz, and Tygon® are used in the train.

Table 4. A summary of methods to analyse chromium samples.

Sample Matrix	Preparation	Analytical Method	Sample Detection Limit	% Recovery	Reference
Air	Sample collected on sodium carbonate-impregnated cellulose filter leached with sodium bicarbonate	Ion chromatography/ Colorimetric	0.1 ng/m^3 30.2 for 20 m^3 sample	89 - 99% at 100 ng	CARB, 1990[7]
Air	Samples collected on filters containing sodium bicarbonate at 15 l/minute	Ion chromatography/ Colorimetric	0.01 ng/m^3 30.2 for 20 m^3 sample	94%	Sheehan et al, 1992[8]
Air: Soluble Cr6+ in: -Plating mists, or Air in absence of reducing agents	Samples collected on alkali-treated PVC/A filters, wet wash with dilute sulphuric acid. Solution mixed with 1,5-diphenylcarbazide solution	Colorimetric	0.025 - 0.12 mg Cr/m^3 for 120 litre air sample	80% at 3 µg/filter	MDHS 52/2 (HSE 1990)[9]
Air: Soluble Cr6+ in absence of reducing agents	Samples collected on alkali-treated PVC/A filters, wet wash with dilute sulphuric acid. Solution mixed with 1,5-diphenylcarbazide solution.	Colorimetric	0.05 µg/sample	Varies with filter batch	NIOSH 1994 (Method 7600) [10]
Air: Soluble and insoluble Cr6+ or Cr6+ in presence of reducing agents e.g. Fe and Fe2+	Samples collected on alkali-treated PVC/A filters, extraction with alkaline solution of NaOH (2%) and $NaCO_3$ (3%). Solution mixed with sulphuric acid and then 1,5-diphenylcarbazide solution.	Colorimetric	0.05 µg/sample	Varies with filter batch	NIOSH 1994 (Method 7600) [10]
Air: soluble and insoluble Cr6+	Sample collected on mixed cellulose ester or glass fibre filter. Wash with distilled water if only soluble Cr6+ to be measured. For both soluble and insoluble Cr6+, extraction with NaOH (2%) and $NaCO_3$ (3%).	Ion chromatography method	3.5 µg/sample	No data	NIOSH 1994 (Method 7604) [11]

4. ATMOSPHERIC DISPERSION MODELLING

Dispersion models compute ambient concentrations as a function of source configurations, emission strengths and meteorological characteristics, thus providing a useful tool to ascertain the spatial and temporal patterns in the ground level concentrations arising from the emissions of various sources. Increasing reliance has been placed on concentration estimates from models as the primary basis for environmental and health impact assessments, risk assessments and emission control requirements. It is therefore important to carefully select a dispersion model for the purpose.

The Appendix contains a discussion on three of the USA-EPA's (and perhaps worldwide) most used dispersion models. These models include the Industrial Source Complex Short Term model (ISCST3), the AERMOD and the CALMET/CALLPUFF suite of models. The selection between the models should be based on the size of the modelling domain and the complexity of the terrain. If a region larger than 50 km by 50 km or in the case of very complex topography, it is recommended that the CALMET/CALPUFF suite of models be used. It is important that the modelling domain must include upper air data. This may result in increasing the domain until such locations are accommodated. If, on the other hand, a fairly small, uncomplicated area is included in the modelling domain, either the ISCST3 or AERMOD could be used. The enhanced model developments included in the AERMOD model, however, makes it a better selection.

The ISCST3 model typically produces predictions within a factor of 2 to 10 within complex topography with a high incidence of calm wind conditions. When applied in flat or gently rolling terrain, the USA-EPA[12] considers the range of uncertainty of the ISCST3 to be -50% to 200%. CALPUFF predictions have been found to have a greater correlation with observations, with more predictions within a factor of 2 of the observations when compared to the ISCST3 model.

The comparison of AERMOD concentrations to ISCST3 concentrations will vary considerably depending on the source configuration, meteorological conditions and terrain influences. Based on evaluations performed during development of AERMOD and consequence analyses comparing ISCST3 and AERMOD, some general conclusions can be drawn, such as:

- AERMOD tends to predict significantly lower concentrations than ISCST3 for complex terrain impacts from elevated sources;
- AERMOD tends to predict lower concentrations than ISCST3 for shorter stacks (less than 20 meters) in rural conditions; and
- The ratio of AERMOD to ISCST3 concentrations tends to increase as the length of the averaging period increases for sources in rural flat terrain.

There will always be some error in any geophysical model, but it is desirable to structure the model in such a way to minimise the total error. The total uncertainty can be thought of as the sum of three components: the uncertainty due to errors in the model physics; the uncertainty due to data input errors; and the uncertainty due to stochastic processes (turbulence) in the atmosphere. The data input uncertainty includes all errors or uncertainties in data such as source variability, observed concentrations, and meteorological data. Even if the field instrument accuracy is excellent, there can still be large uncertainties due to unrepresentative placement of the instrument (or taking of a sample for analysis). It is well known that wind direction errors are the major cause of poor agreement, especially for relatively short-term predictions (minutes to hourly) and long downwind distances. However, model evaluation studies suggest that the source data input error term is often the major contributor to total uncertainty. Even in the best tracer studies, the source emissions are known only with an accuracy of ±10%, which translates directly into a minimum error of that magnitude in the model predictions.

All of the above factors contribute to the inaccuracies not even associated with the mathematical models themselves. Determining the impact of air pollutants when already dilute at its origin is not necessarily a trivial task. Apart from the difficulty in measuring the rate of emission, care must be taken when employing off-the-shelf atmospheric dispersion models under these situations. Air pollution emissions are most frequently treated as so-called "point sources", which assumes that the total source consists of the pollutant of concern (i.e. 100%). This can be shown as a fair assumption even when the pollutant concentration is as low as a percentage of the total flow, provided the calculation distance is not too close to the source – typically further than 100m. It is not even uncommon for point sources to be assumed with pollutant concentrations of the order of 0.01% of the total emission. However, when dealing with emissions with concentrations of 0.001% and less, the error (i.e. over estimating the concentrations) can be a few factors, depending on the atmospheric conditions.

This is illustrated by way of an example, using the emission factors given in Table 3. For an annual ferrochromium production 45 000 tons, the particulate rate from an open furnace bag house, would is estimated to be 0.2 g/s. Similarly, total chromium and hexavalent chromium emission rates would be 2 mg/s and 0.09 mg/s, respectively. Whilst the particulate matter concentration in the source is typically 1 to 10 mg/Nm^3, the hexavalent concentration would be 0.0004 to 0.004 mg/Nm^3. The latter represents concentrations of between 0.00004% and 0.0004% of the total flow.

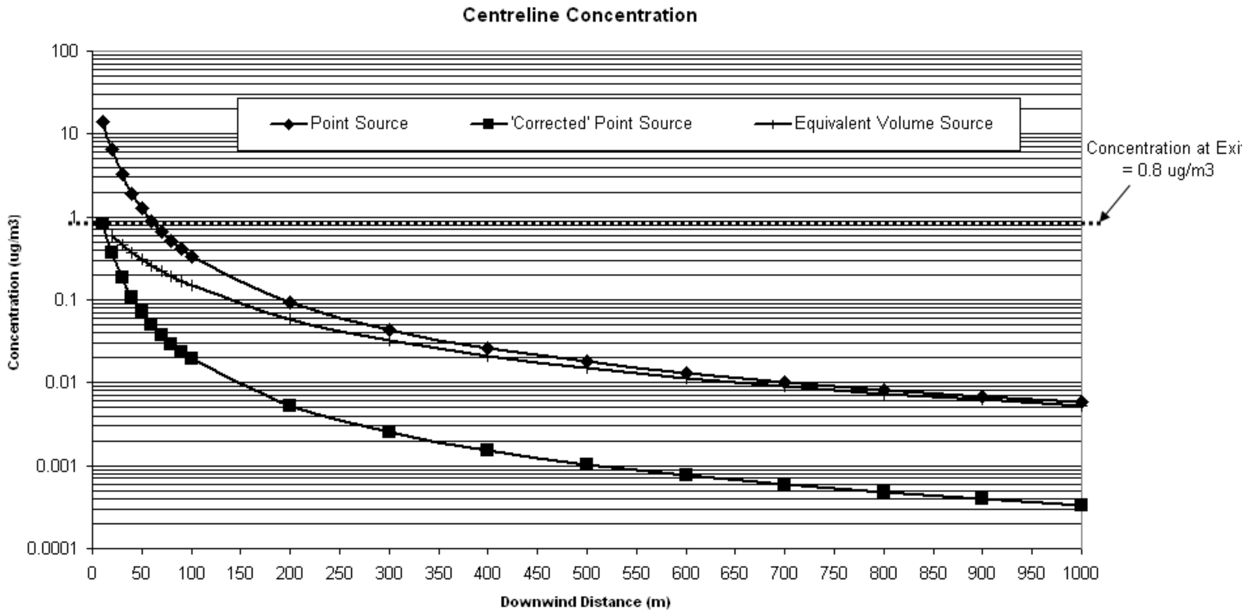

Figure 2. Predicted downwind concentrations of dilute hexavalent chromium emission.

Assuming a point source, and using a Gaussian dispersion model, such as the ISCST3 or their AERMOD model, it can be shown that the resulting hexavalent chromium concentrations could be over-predicted by between 4 and 35 times during stable night time conditions. During daytime unstable or neutral, windy conditions this error becomes less – the worst over-prediction occurring during calm, unstable conditions, i.e. an 8-fold error with the lower hexavalent concentration of 0.00004%. In reality, this over-prediction is more likely to occur near the source, and very little difference is expected at distances of 1km and further.

The example shown in Figure 2 is for a very stable, night time atmosphere. The particulate concentration at source is 2 mg/Nm^3, and for hexavalent chromium, 0.8 µg/Nm^3. The top curve represents the assumption of a simple point source, whereas the bottom curve represents the point source prediction corrected to provide a concentration of 0.8 µg/Nm^3 near the source.

The third curve represents the emission as an initial “volume source” resulting in a concentration of 0.8 µg/Nm^3 near the point of emission. By defining the source as a “volume source”, the model treats the initial part of the plume as if it were further downwind, thus providing the enhanced dilution required to represent the dilute emission at source. This source configuration clearly illustrates a more realistic treatment of dilute emissions such as those at bag houses.

5. CANCER RISK

The US Agency for Toxic Substances and Disease Registry (ATSDR), Health Canada, US Environmental Protection Agency (USA EPA), and the World Health Organisation (WHO) have evaluated the cancer inhalation toxicity data for hexavalent chromium.

Based on an occupational exposure study of chromate workers, the USA EPA has classified hexavalent chromium as a known human carcinogen and calculated an air unit cancer risk factor of 1.2×10^{-2} per µg/m^3, that is an excess risk for lung cancer of 12 persons in 1 000 exposed to 1 µg/m^3 throughout their lifetime. Health Canada used a different approach in interpreting data from the same study as USA EPA did, and derived a unit cancer risk factor of 8.0×10^{-2} $(\mu g/m^3)^{-1}$. WHO presented the unit cancer risk factor as the range 1.1 to 13 x 10^{-2} $(\mu g/m^3)^{-1}$.

6. CONCLUSIONS

Hexavalent chromium is classified as Group A - known human carcinogen by the inhalation route of exposure, but that carcinogenicity by the oral route of exposure cannot be confirmed and in that regard it is classified as Group D. Trivalent chromium is not classified as a human carcinogen, based on the grounds that there are inadequate data to determine the potential carcinogenicity.

Preliminary emission factors for hexavalent chromium are presented for the South African ferrochrome industry. The smelting of chromium in the electric arc furnace is the major source of chromium emissions in a ferrochromium plant. Open furnaces have the highest uncontrolled chromium emissions. These emissions are normally routed to cyclones followed by bag filters. Wet scrubbers are used exclusively to control exhaust gases from closed furnaces. Although the emissions from the scrubbers have an insignificant content of hexavalent chromium, the combustion of the carbon monoxide-rich gas in the heating and sintering processes, and the burning of the excess gas in the flare could potentially generate more significant levels of hexavalent chromium.

The following two sampling and analytical methods for source characterisation are recommended:

- USEPA Method 0012 (Metals)
- Method Cr+6

Laboratory techniques need to have detection limits well below the methods normally used for occupational hygiene exposures.

The discussion on dispersion models was limited to three dispersion models only, namely:

- The US EPA's Industrial Source Complex Model (Version 3);
- The CALMET/CALPUFF models; and,
- The AERMET/AERMOD suite of models.

Careful consideration needs to be taken when selecting a dispersion model. Factors affecting this selection include topographical features, the presence of large water masses, the size of the impact area under investigation and the source configurations.

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APPENDIX

The Industrial Source Complex Model (ISCST3)

The Industrial Source Complex Short Term model (ISCST3) model is included in a suite of models used by the US-EPA for regulatory purposes. ISCST3 is a steady state Gaussian Plume model, which is applicable to multiple point, area and volume sources. Gently rolling topography may be included to determine the depth of plume penetration by the underlying surface. A disadvantage of the model is that spatial varying wind fields, due to topography or other factors cannot be included. A further limitation of the model arises from the models treatment of low wind speeds. Wind speeds below 1 m/s produce unrealistically high concentrations when using the Gaussian plume model, and therefore all wind speeds below 1 m/s are simulated using 1 m/s.

Input data types required for the model include: source data, meteorological data, terrain data and information on the nature of the receptor grid. ISCST3 requires hourly average meteorological data as input, including wind speed, wind direction, a measure of atmospheric turbulence, ambient air temperature and mixing height.

When building influence is suspected, the effect of downdraft must be taken into account. The flow characteristics of air moving over the furnace buildings may induce a downwash on the leeward side, drawing the plume to the ground near the source. Building down-wash algorithms have been developed for air quality dispersion models such as the ISCST3. These algorithms require additional input to be prepared and included in the model runs. The Building Profile Input Program (BPIP) was applied in the determination of whether or not each of the stack's plumes were subject to structure wake effects, and for the preparation of ISCST3 model input.

The AERMOD Model

The AERMOD model has been developed by the American Meteorological Society/Environmental Protection Agency Regulatory Model Improvement Committee (AERMIC).

The modelling system consists of three separate components: AERMOD (AERMIC Dispersion Model), AERMET (AERMOD Meteorological Pre-processor), and AERMAP (AERMOD Terrain Pre-processor). The development effort, which began in 1991, was undertaken to introduce state-of-the-art modelling concepts into the EPA's air quality models. The focus of AERMIC was on upgrading regulatory steady-state plume modelling to incorporate air dispersion based on planetary boundary layer turbulence structure and scaling concepts, including treatment of both surface and elevated sources, and both simple and complex terrain. The implementation and evaluation of the improved building downwash algorithms from the ISC-PRIME model into AERMOD have recently been completed.

AERMOD can be used to model impacts from point, volume, and area sources. Area sources can be defined as rectangular, circular or as an irregularly shaped polygon. The model does not currently support deposition algorithms.

AERMOD includes a continuous treatment for characterizing dispersion based on similarity theory, as compared to ISCST3's use of discrete stability classes. The Monin-Obukhov length (L) is used as the stability parameter, and is computed by the AERMET meteorological pre-processor. This is one of the significant improvements in AERMOD's formulation as compared to the ISCST3 model.

Multiple levels of wind, temperature and turbulence data can be input to the modelling system. The wind and turbulence data may come from SODAR measurements or from an instrumented tower. The AERMET meteorological processor also requires at least one wind measurement at or below 100 meters for use in boundary layer scaling.

AERMOD can be considered an "all terrain" model. It applies to all terrain situations, including flat terrain applications, as well as terrain above stack base (elevated terrain) and terrain above stack height (complex terrain). However, there is no distinction made in AERMOD between elevated simple terrain and complex terrain, as in the ISCST3 model. Instead, the AERMOD terrain algorithm provides a continuous treatment of terrain influences across the stack height demarcation. As a result, there is no need for intermediate terrain processing as performed in the ISCST3 model. The model, does not construct a three-dimensional wind field such as the CALMET model (see next section).

The CALMET/CALPUFF Model

The Industrial Source Complex and AERMOD models are based on steady-state plume assumption, with meteorological inputs assuming a horizontally-uniform flow field. Usually the winds are derived from a single point measurement, which is often made at a nearby non-complex terrain site. The steady-state flow fields do not reproduce the terrain-induced spatial variability in the wind field. In addition to which, the straight-line trajectory assumption of the plume models cannot easily handle curved trajectories associated with terrain-induced deflection or channelling. These limitations of plume models can significantly affect the model's ability to correctly represent the spatial area of impact from sources in complex terrain, in addition to the magnitude of the peak values in certain instances[13].

In general, the differences between CALPUFF and ISCST3/AERMOD concentration results are caused by how emissions are transported and dispersed. CALPUFF limits downwind transport based on the wind speed while there is no such limitation in ISCST3 (it is a plume model). Under calm wind conditions, CALPUFF continues to disperse each puff while the ISCST3 model is arbitrarily set not to determine concentrations when wind speeds are less than 1 m/s. CALPUFF is capable of tracking the puff emitted before, during and after wind shifts and reversals while ISCST3 is only concerned with the current hour transport of its plume(s). CALPUFF continues to disperse each puff even when they are above an inversion layer while ISCST3 determines its plume is above the inversion layer and cannot be advected to the ground.

CALPUFF requires as a minimum, the input of hourly average surface meteorological data. However, in order to take full advantage of the model's ability to simulate spatially varying meteorological conditions and dispersion within the convective boundary layer it is necessary to generate a three-dimensional wind field for input to the CALPUFF model. The CALMET model may be used to generate such a three-dimensional wind field for input to the CALPUFF model.

The CALMET meteorological model contains a diagnostic wind field module that includes parameterised treatments of terrain effects, including slope flows, terrain channelling and kinematic effects, which are responsible for highly variable wind patterns. The CALMET model also comprises boundary layer models for application to overland and overwater areas.

By using CALMET and CALPUFF in combination, it is possible to treat many important complex terrain effects, including spatial variability of the meteorological fields, curved plume trajectories and plume-terrain interaction effects. Maximum hourly average, highest daily average and annual average concentrations for particulate and gaseous emissions will be simulated through the application of CALPUFF, using as input the relevant emissions data and the three-dimensional CALMET data set.